IOWA STATE UNIVERSITY
Digital Repository

Retrospective Theses and Dissertations

Iowa State University Capstones, Theses and Dissertations

1958

Structures of some hydrated rare earth ethylsulfates

Donald Robert Fitzwater
Iowa State College

Follow this and additional works at: https://lib.dr.iastate.edu/rtd

 Part of the Physical Chemistry Commons

Recommended Citation
Fitzwater, Donald Robert, "Structures of some hydrated rare earth ethylsulfates " (1958). *Retrospective Theses and Dissertations*. 1629.
https://lib.dr.iastate.edu/rtd/1629

This Dissertation is brought to you for free and open access by the Iowa State University Capstones, Theses and Dissertations at Iowa State University Digital Repository. It has been accepted for inclusion in Retrospective Theses and Dissertations by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.

www.manaraa.com

STRUCTURES OF SOME HYDRATED RARE EARTH ETHYLSULFATES

by

Donald Robert Fitzwater

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Major Subject: Physical Chemistry

Approved:

Signatures have been redacted for privacy.

Iowa State College
1958

TABLE OF CONTENTS

		Page
I.	INTRODUCTION	1
	A. Structural Interest	1
	1. Crystalline fields and spectra	1
	2. The Jahn-Teller effect	2
	3. Previous structural investigation	3
	B. Methods of Computation	5
	1. Computation requirements	5
	2. The I.B.M. 650	6
II.	COMPUTATIONAL METHODS	8
	A. Evaluation of the Fourier Series	8
	1. General problem	8
	2. Three dimensional block program	19
	3. Block peak program	22
	4. The T.D.F. 40-80 program	22
	B. Least Squares Method	25
	1. General problem	25
	2. L.S.II program	31
	3. L.S.II M program	33
III.	STRUCTURAL DETERMINATIONS	35
	A. Structure of $Er(C_2H_5SO_4)_3 \cdot 9H_2O$	35
	1. Data	35
	2. Trial structure	38
	3. Refinement of the trial structure	41
	B. Structure of $Y(C_2H_5SO_4)_3 \cdot 9H_2O$	49
	1. Data	49
	2. Refinement of the trial structure	52
	C. Structure of $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$	57
	1. Data	57
	2. Refinement of the trial structure	58

TABLE OF CONTENTS (Continued)

		Page
	D. Discussion of Structures	59
	1. Coordination of the rare earth ion	59
	2. The ethylsulfate ion structure	63
	3. The position of hydrogen bonds	64
	4. The Jahn-Teller effect	67
IV.	SUMMARY	68
	A. Computing Methods	68
	B. Structure Determination	68
V.	BIBLIOGRAPHY	70
VI.	ACKNOWLEDGMENTS	72
VII.	APPENDIX A: T.D.F. 80 B PROGRAM	73
	A. Fourier Series Evaluation for a 4x4x4 Point Block	73
	1. Mathematical method	73
	2. Range and accuracy	76
	3. Storage	76
	4. Speed	76
	5. Equipment specifications	76
	6. Error checks	76
	7. Input-output	77
	8. Symmetry provisions	77
	B. Detailed Operating Instructions	78
	1. Detail cards	78
	2. Special information cards	79
	3. Program loading cards	81
	4. Output cards	82
	5. Operating procedure	83
	6. Flow diagram, program cards, and wiring diagram	84
VIII.	APPENDIX B: T.D.F. 40-80 PROGRAM FOR I.B.M. 650	98
	A. Fourier Series Evaluation on a Grid Spacing of 1/40 or 1/80 of the Unit Cell	98

TABLE OF CONTENTS (Continued)

		Page
	1. Function to be evaluated	98
	2. Method of evaluation	99
	3. Method of expansion	100
	4. Flow diagram, wiring information, and speed	103
B.	Operating Instructions	103
	1. Card formats	103
	2. Assembly of program deck	110
	3. Tabulation	112
	4. Empty drum cells	112
	5. Control card formats	113
	6. The program deck	116
IX.	APPENDIX C: L.S.II M PROGRAM	134
A.	Form of the L.S.II M Program	134
	1. Modifications made to L.S.II	134
	2. Programming information	135
B.	Operating Instructions	138
	1. Assembly of input deck	138
	2. Console operation	139
	3. Subsequent cycles	139
	4. Description of input cards	140
	5. Description of output cards	143
	6. Plug board	144
	7 Program deck	144
X.	APPENDIX D: STRUCTURE FACTORS	154

I. INTRODUCTION

A. Structural Interest

1. Crystalline fields and spectra

The spectra arising from an ion in a crystal are usually composed of diffuse lines or bands. The reason for this is the strong perturbation of the energy levels of the ion by the instantaneous crystalline field.

The rare earth ions in a crystal, having 4f electrons shielded from field fluctuations by a closed 5 s^2p^6 shell, give sharp spectra. An averaged field does penetrate and cause splitting and shifting of the ions' 4f energy levels. Consequently, these spectra contain information about the crystalline field, and the electronic structure of the ion. If the electronic structure of the ion is known, the crystalline fields can be studied. The splitting of degenerate energy levels and the transition selection rules are dependent upon the field symmetry about the ion. Such an analysis has been made for europium ethylsulfate nonahydrate by E. V. Sayre and S. Freed (1). The symmetry about the rare earth ion used in this investigation was D_{3h} for the water molecules and C_{3h} for the complete environment. These symmetries were obtained from the work of J. A. A. Ketelaar which will be discussed later in this chapter.

The paramagnetic resonance spectra of gadolinium and neodymium ethylsulfates have been studied by B. Bleaney, H. E. D. Scovil, and R. S. T. Trenam (2). The results are consistent with an ion symmetry of C_{3h} except for some discrepancies in the position of the zero field lines. The origin of these discrepancies is not clear. Work on other magnetic properties of the rare earth salts is being carried out by R. M. Bozorth (3).

Active investigations of the magnetic properties, heat capacities and spectra of the rare earth ethylsulfates are being carried out by F. H. Spedding and co-workers (4). The accurate spectra obtained in this work will enable a careful and thorough analysis of the crystalline field perturbations in the excited as well as in the ground state.

One of the reasons for this present investigation is to furnish an accurate structure for the ethylsulfate compounds so that the symmetry of the water molecules about the rare earth ion will be known. In addition, if field strengths are to be computed, the positions of the sulfate oxygens and the orientation of the water dipoles must be known. This information can be obtained from a careful study of the crystals by X-ray diffraction.

2. The Jahn-Teller effect

It was shown by H. A. Jahn and E. Teller (5) that a configuration of a polyatomic molecule for an electronic state

having orbital degeneracy cannot be stable with respect to all displacements of the nuclei unless, in the original configuration, the nuclei all lie on a straight line. If electronic spin degeneracy is also included (6), the degenerate nonlinear configuration can be stable only if the degeneracy is of the Kramers type (7), which can occur only if the molecule contains an odd number of electrons. Consequently, the stable state of such a system must be asymmetric enough to split the degeneracy of the ground state.

The structures of the titanium and vanadium alums were discussed by J. H. VanVleck (8), (9) and the size of the distortions of the coordinated water molecules produced by the Jahn-Teller effect was predicted to be about 10^{-9} cm. The distortions which would be expected in the case of the rare earth ions were predicted to be about 10^{-11} cm. Such differences could be detected in the case of the alums but the distortions expected for the rare earth compounds are too small to be detected at the present state of the art of X-ray diffraction. However, a careful structure determination would place an upper limit on such distortions and could verify experimentally that the distortions were indeed quite small.

3. Previous structural investigation

The structures of the rare earth ethylsulfate hydrates have been studied by J. A. A. Ketelaar (10), who determined the lattice constants of many of these compounds with an error

of ± 0.003 Å in a and of ± 0.01 Å in c. The compounds were found to be isomorphous within experimental error. The most probable space group was given as C_{6h}^2 - $P6_3/m$ with other possible choices of C_6^6 - $P6_3$ and C_{3h}^1 - $P\bar{6}$. A careful discussion of the symmetry about the rare earth ion was given, with the conclusion that the symmetry was almost certainly C_{3h}.

The rare earth ions were found to be in the special position 1/3, 2/3, 1/4 and 2/3, 1/3, 3/4. The sulfur was found to be in a six-fold set with the parameters 0.35, 0.02, 0.25. The sulfate oxygens were assigned to two six-fold sets and one twelve-fold set and approximate parameters were given so as to produce a tetrahedron of oxygens about each sulfur. The parameters of the carbon atoms and water molecules were not given, but, from packing considerations, a structure was postulated. This structure places nine water molecules about the rare earth ion and one of the two six-fold sulfate oxygens in the mirror plane of the rare earth ion at a distance of 2.90 Å.

In view of the available techniques for evaluating structures at that time, it was not practical to continue the structural determination. One of the reasons for the present work is to check and complete the above structural determination.

B. Methods of Computation

1. Computation requirements

The determination of the structure of a moderately complex crystal may require many evaluations of certain Fourier series and a refinement of the model so obtained by the use of a least squares technique.

The Fourier series representing either the electron density or the Patterson function is usually evaluated on a lattice containing from six thousand to five hundred thousand points. The series itself may contain from two hundred to several thousand terms. It can be seen that hand computation is feasible only in the smallest cases and is practically impossible in the more general cases.

The least squares refinement of a moderately complex model may require the fitting of from two hundred to several thousand pieces of data to from twenty to fifty parameters related to the data through a set of trigonometric equations. For small quantities of data and few parameters, hand computation is quite feasible but, in the more extensive cases, the labor and the errors involved in hand computation prohibit the use of the method.

These computations are almost ideally suited for evaluation by large scale digital computers. Because of limitations on the speed and memory capacity of currently available computers, and because the computations must be economically

justified, much care must be used in setting up such problems for the computing machines. The method to be used or the form and nature of the answers to be obtained must be adjusted to these demands.

2. The I.B.M. 650

The Type 650 Magnetic Drum Data-Processing Machine manufactured by the International Business Machine Corporation, commonly abbreviated the I.B.M. 650, is a medium sized digital computer using a magnetic drum memory system. This general purpose computer has storage facilities for 2000 "words" on a magnetic drum. Each word is an order or a ten digit number with sign. Each of the 2000 locations is assigned a four digit address of 0000 to 1999. The input and output for the basic machine is in the form of punched cards. For further information please refer to the instruction manual for the I.B.M. 650 (11). The advent of this machine on campus has made it possible to carry out the calculations described above on a routine basis. It is not large enough nor fast enough to handle the very complex crystals but it can handle all moderately complex problems in an economical manner. It should be pointed out that the reasons the very complicated problems are not feasible are essentially economic. A larger machine can carry out such calculations economically. Provided the problems are broken up properly, such calculations can be

carried out on the I.B.M. 650 in a matter of a few days if the resulting expense is acceptable.

Many crystallographers have access to this computer and the interest in obtaining crystallographic programs for the I.B.M. 650 is high. Many crystallographic programs have been and are being written and the program library is large enough so that the application of the normal methods of structure analysis becomes almost routine. Information as to the availability of crystallographic programs is available either from the International Business Machines Corporation or from the Computation and Data Processing Center of the University of Pittsburgh.

Since there existed a need for several programs which were not available, it was felt that it would be both interesting and useful to write the required programs. During the course of this work it was found convenient to modify the excellent least squares program, L.S.II (12) which was already available.

The greatest lack of programs seemed to lie in the area of Fourier series evaluation. Consequently, the programming effort was designed to remedy this lack. Because of the limitations of the I.B.M. 650, much thought was given to the problem of adapting the computation method and the form of the output to the I.B.M. 650.

II. COMPUTATIONAL METHODS

A. Evaluation of the Fourier Series

1. General problem

The electron density in the unit cell of a crystal can be represented as a three dimensional Fourier series (13). This series takes the form

$$(1)\quad \rho(x,y,z) = 1/V \sum_{hk\ell=-\infty}^{\infty} F(hk\ell)\ \exp -2\pi i(hx/a + ky/b + \ell z/c)$$

where $\rho(x,y,z)$ is the electron density, $F(hk\ell)$ is the structure factor for the reflection $(hk\ell)$, V is the volume of the unit cell and a,b,c, are the unit cell dimensions. In the normal case of a mosaic crystal, the intensity of the $(hk\ell)$ reflection is proportional to the square magnitude of the structure factor. All information as to the phase angle of the reflection is lost when the intensity of the reflection is recorded. This information must be recovered by the use of a trial model for the structure, by the use of the Patterson function discussed below, or by some other means. There are some more direct methods for solving the phase problem, but they will not be discussed here. The phase angle calculated on the basis of the trial model can be used to assign a phase angle to the observed magnitudes of $F(hk\ell)$. The

series (1) can then be summed. The resulting electron density can be compared with the model used. If the model is correct the electron density will agree except for series termination errors. This error arises from the termination of the series after a finite number of terms. If the electron density does not agree with the model, a new model is required. If, as is usually the case, the electron density agrees with the model in some important features but disagrees or supplements the model in other features, modification of the model and recalculation of the electron density may lead to convergence on the correct model.

The Fourier series, in somewhat different form, may lend more direct assistance in obtaining a suitable model. The function

$$(2)\quad P(x,y,z) = 1/V \sum_{\substack{hk\ell \\ -\infty}}^{\infty} |F(hk\ell)|^2 \exp -2\pi i(hx/a + ky/b + \ell z/c)$$

which uses only coefficients which are directly related to the observed intensities is known as the Patterson function (14). This function can be interpreted as having a maximum at those points which correspond to the end point of some interatomic vector referred to the origin of the unit cell. Because of the large number of such maxima, this function rarely can be interpreted to give a complete model. In many cases, however, at least some of the more important features of the model can

be obtained. The problem of the evaluation of such series is essentially the same as the problem of the evaluation of the electron density function.

The above discussion is not intended to be complete. There are other techniques utilizing Fourier series which are useful, but which involve the same computational problem.

If the wave length of the X-radiation is not too close to an absorption edge of a crystal component, Freidel's law (15), which states that $F(hk\ell)$ is the conjugate of $F(\bar{h}\bar{k}\bar{\ell})$, will hold. The notation $\bar{h}\bar{k}\bar{\ell}$ means -h, -k, and $-\ell$. By using the expressions $F(hk\ell) = A(hk\ell) + iB(hk\ell) = F^{*}(\bar{h}\bar{k}\bar{\ell}) = A(\bar{h}\bar{k}\bar{\ell}) - iB(\bar{h}\bar{k}\bar{\ell})$ and $\theta(hk\ell) = 2\pi(hx/a + ky/b + \ell z/c)$ the electron density can be written as

$$
\begin{aligned}
(3)\ \rho(x,y,z) = 2/V \sum_{\substack{hk\ell \\ 1}}^{\infty} \Big[& A(hk\ell)\cos\theta(hk\ell) + B(hk\ell)\sin\theta(hk\ell) \\
& + A(\bar{h}\bar{k}\ell)\cos\theta(\bar{h}\bar{k}\ell) + B(\bar{h}\bar{k}\ell)\sin\theta(\bar{h}\bar{k}\ell) \\
& + A(h\bar{k}\ell)\cos\theta(h\bar{k}\ell) + B(h\bar{k}\ell)\sin\theta(h\bar{k}\ell) \\
& + A(\bar{h}k\ell)\cos\theta(\bar{h}k\ell) + B(\bar{h}k\ell)\sin\theta(\bar{h}k\ell)\Big] \\
+ 2/V \sum_{\substack{k\ell \\ 1}}^{\infty} \Big[& A(0k\ell)\cos\theta(0k\ell) + B(0k\ell)\sin\theta(0k\ell) \\
& + A(0\bar{k}\ell)\cos\theta(0\bar{k}\ell) + B(0\bar{k}\ell)\sin\theta(0\bar{k}\ell)\Big] \\
+ 2/V \sum_{\substack{h\ell \\ 1}}^{\infty} \Big[& A(h0\ell)\cos\theta(h0\ell) + B(h0\ell)\sin\theta(h0\ell) \\
& + A(\bar{h}0\ell)\cos\theta(\bar{h}0\ell) + B(\bar{h}0\ell)\sin\theta(\bar{h}0\ell)\Big]
\end{aligned}
$$

$$+ 2/V \sum_{\substack{hk \\ l}}^{\infty} \left[A(hk0) \cos \theta(hk0) + B(hk0) \sin \theta(hk0) + A(h\bar{k}0) \cos \theta(h\bar{k}0) + B(h\bar{k}0) \sin \theta(h\bar{k}0)\right]$$

$$+ 2/V \sum_{\substack{h \\ l}}^{\infty} \left[A(h00) \cos \theta(h00) + B(h00) \sin \theta(h00)\right]$$

$$+ 2/V \sum_{\substack{k \\ l}}^{\infty} \left[A(0k0) \cos \theta(0k0) + B(0k0) \sin \theta(0k0)\right]$$

$$+ 2/V \sum_{\substack{\ell \\ l}}^{\infty} \left[A(00\ell) \cos \theta(00\ell) + B(00\ell) \sin \theta(00\ell)\right]$$

$$+ 1/V \, A(000).$$

This particular expression is derived in a form containing only positive values of ℓ for convenience in adapting to the I.B.M. 650 program.

If we include the special reflections (those containing one or more zero indices) in the general form, they must be divided by a multiplicity factor of 2^N where N is the number of zero indices occurring in $F(hk\ell)$. If we define $F'(hk\ell) = \frac{2^{1-N}}{V} F(hk\ell)$, the summation now becomes

$$(4)\ \rho(x,y,z) = \sum_{\substack{hk\ell \\ 0}}^{\infty} \Big[A'(hk\ell) \cos \theta(hk\ell) + B'(hk\ell) \sin \theta(hk\ell)$$
$$+ A'(\bar{h}\bar{k}\ell) \cos \theta(\bar{h}\bar{k}\ell) + B'(\bar{h}\bar{k}\ell) \sin \theta(\bar{h}\bar{k}\ell)$$
$$+ A'(h\bar{k}\ell) \cos \theta(h\bar{k}\ell) + B'(h\bar{k}\ell) \sin \theta(h\bar{k}\ell)$$
$$+ A'(\bar{h}k\ell) \cos \theta(\bar{h}k\ell) + B'(\bar{h}k\ell) \sin \theta(\bar{h}k\ell) \Big].$$

By using the trigonometric identities,

$$\cos \theta(hk\ell) = \cos \theta(h00) \cos \theta(0k0) \cos \theta(00\ell)$$
$$- \cos \theta(h00) \sin \theta(0k0) \sin \theta(00\ell)$$
$$- \sin \theta(h00) \cos \theta(0k0) \sin \theta(00\ell)$$
$$- \sin \theta(h00) \sin \theta(0k0) \cos \theta(00\ell)$$

and,

$$\sin \theta(hk\ell) = \sin \theta(h00) \cos \theta(0k0) \cos \theta(00\ell)$$
$$+ \cos \theta(h00) \sin \theta(0k0) \cos \theta(00\ell)$$
$$+ \cos \theta(h00) \cos \theta(0k0) \sin \theta(00\ell)$$
$$- \sin \theta(h00) \sin \theta(0k0) \sin \theta(00\ell)$$

the expression for the electron density becomes, in expanded form,

$$(5)\ \rho(x,y,z) = \sum_{\substack{hk\ell \\ 0}}^{\infty} \Big[A_1(hk\ell) \cos \theta(h00) \cos \theta(0k0) \cos \theta(00\ell)$$
$$+ A_2(hk\ell) \sin \theta(h00) \sin \theta(0k0) \cos \theta(00\ell)$$

$$
\begin{aligned}
&+ A_3(hk\ell)\ \sin\theta(h00)\ \cos\theta(0k0)\ \sin\theta(00\ell) \\
&+ A_4(hk\ell)\ \cos\theta(h00)\ \sin\theta(0k0)\ \sin\theta(00\ell) \\
&+ B_1(hk\ell)\ \sin\theta(h00)\ \sin\theta(0k0)\ \sin\theta(00\ell) \\
&+ B_2(hk\ell)\ \cos\theta(h00)\ \cos\theta(0k0)\ \sin\theta(00\ell) \\
&+ B_3(hk\ell)\ \cos\theta(h00)\ \sin\theta(0k0)\ \cos\theta(00\ell) \\
&+ B_4(hk\ell)\ \sin\theta(h00)\ \cos\theta(0k0)\ \cos\theta(00\ell)\Big].
\end{aligned}
$$

The A_i and B_i are linear combinations of $A'(hk\ell)$ and $B'(hk\ell)$ respectively.

These expressions are

$$
\begin{aligned}
A_1 &= A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_2 &= -A'(hk\ell) - A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_3 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) - A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_4 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) - A'(\bar{h}k\ell) \\
B_1 &= -B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_2 &= B'(hk\ell) + B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_3 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) - B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_4 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) - B'(\bar{h}k\ell)
\end{aligned}
\tag{6}
$$

The space group of the crystal introduces other symmetry and creates relationships among the $A(hk\ell)$ and the $B(hk\ell)$ that usually simplify the above expressions. It should be noted that, if the space group possesses a center of symmetry, $F(hk\ell) = F(\bar{h}\bar{k}\bar{\ell})$. But Friedel's Law states that $F(hk\ell) = F^*(\bar{h}\bar{k}\bar{\ell})$, and so we must have all $B(hk\ell) = 0$.

There are two general methods for evaluating such series; one is to evaluate the series directly as a three dimensional sum in the form (4) or (5), the other is to use form (5) and to evaluate it as successive one dimensional summations. In general, it can be said that the calculation time required for successive one dimensional summations is relatively independent of the number of terms to be summed provided the symmetry is unchanged, while the direct evaluation is essentially proportional to the number of terms to be summed. The intermediate results which must be retained are much more extensive in the first case than in the second. It can be seen that the best form is strongly dependent upon the specifications of the computer to be used and the number of terms to be considered. In general, provided the requirements for moderately fast large capacity storage can be met, it would appear better to do full calculations in the expanded form and partial calculations of correction terms in the unexpanded form. The correction results could be added to the previous results to give the new function.

Another point, which is of great interest, is the possibility of evaluating such series only over the basic 1/64 of the unit cell (1/4 x 1/4 x 1/4). Use can be made of trigonometric relationships to produce the required values in the remainder of the cell. In the case of series (4) this involves breaking the calculation up into groups of terms, each of which transform in the same way. The sums of each group

can then be transformed to give the final result. Unfortunately, this requires a knowledge of the same expression with sin substituted for cos and vice versa. This doubling of work is somewhat unsatisfactory and increases the output data. In addition, the translation of these groups is not very simple. Expansion in each of the three dimensions involves such relations as

$$\begin{aligned}\cos(A + m\pi/2) &= \cos A \text{ if } m = 4n\\ &= -\sin A \text{ if } m = 4n + 1\\ &= -\cos A \text{ if } m = 4n + 2\\ &= \sin A \text{ if } m = 4n + 3\end{aligned}$$

and

$$\begin{aligned}\sin(A + m\pi/2) &= \sin A \text{ if } m = 4n\\ &= \cos A \text{ if } m = 4n + 1\\ &= -\sin A \text{ if } m = 4n + 2\\ &= -\cos A \text{ if } m = 4n + 3\end{aligned}$$

The series (5) can be transformed in a somewhat simpler manner by the relations

$\cos 2\pi hx = \cos 2\pi hx$	$\sin 2\pi hx = \sin 2\pi hx$
$\cos 2\pi h(x+1/4)=(-1)^h\cos 2\pi hx'$	$\sin 2\pi h(x+1/4)=(-1)^{h+1}\sin 2\pi hx'$
$\cos 2\pi h(x+1/2)=(-1)^h\cos 2\pi hx$	$\sin 2\pi h(x+1/2)=(-1)^h\sin 2\pi hx$
$\cos 2\pi h(x+3/4)=\cos 2\pi hx'$	$\sin 2\pi h(x+3/4)= -\sin 2\pi hx'$

where $x' = 1/4 - x$. In the case of an expansion by 1/4 or 3/4, the coordinate corresponding to x in the basic 1/64 of the cell is read in reverse and translated. This is carried out by simply changing the labeling of the points on the final tabulated results.

As a consequence, if the terms of the series are broken up into groups, each with the same translation properties in three dimensions, and the group sums are obtained over the basic 1/64 of the unit cell, the results for the remainder of the cell may be obtained by summing the same groups but with the signs of certain groups changed. This can be carried out automatically at the time of tabulation, even on the I.B.M. 402 tabulator. The proper wiring for any given translation can be selected by three external switches, each controlling the translation in one of the three dimensions. The results of the three independent translations are combined by the use of coselectors to control the addition or subtraction of a given group under the translations set in the switches.

A similar method could be used to expand the results from series (4) but the added complication of having sin and cos type contributions which must be selected would prohibit its use with the I.B.M. 402 tabulator unless these were selected before each translation. The two systems would not be compatible and could not be summed and translated together. Compatibility might be attainable on an I.B.M. 407

tabulator but this has not been investigated. However, if the form (4) is to be used for correction terms only, the most convenient thing to do would probably be to evaluate directly over all of the cell that is of interest. Then if the results were treated as even cos terms, and odd quarters of the unit cell punched in reverse, the corresponding sums for each translation could be added to the original series (5) cards to give the new evaluation of the electron density.

The above treatment of correction terms from series (4) is the most efficient over the basic 1/64 of the unit cell, but duplication becomes comparatively expensive if many such cell fractions must be used. A third procedure, better adapted for many cell fractions but less efficient in the basic 1/64 of the unit cell, is to use series (5) but not to use successive one dimensional summations. By taking advantage of the smaller number of terms, even moderate storage facilities will enable the direct evaluation of the same subseries and the utilization of the same expansion scheme as for the successive one dimensional summations.

There remains one further question to be discussed. That is the question of the nature of the desired final information and the effect of this on the programming. The Fourier series are used both in searching for new features to be included in a model and in improving the parameters of a rough but essentially complete model. In the first case the volume of the unit cell must be completely explored. In

the second case, because of a knowledge of the rough parameters, only a small part of the total unit cell volume really needs to be explored. The three successive one dimensional summations are more suitable for the first case, while small parts of the unit cell can readily be explored by series (4) or by the method discussed above using series (5) without successive summations.

The information in the second case that is really desired is the location of the maximum and the shape of the peak. The results of a limited exploration about the maxima could then be used in a separate program to produce this information. The lattice points must be close enough to accurately define the shape of the peak.

There are three general ways to explore the whole unit cell. One is to evaluate the series on a mesh fine enough to give a satisfactory definition of the peak. The second is to use a rough 'searching' mesh and a fine mesh about each interesting point. The third method is to compute the projection of the electron density onto a plane and then evaluate the electron density along a line perpendicular to each maximum to find the third coordinate. A fine mesh evaluation about this point would then give the desired information. It would appear that, in any given problem, one of the above procedures would be better than any of the others and that, ideally, one would like to be able to use that method which is thought to be best suited. This would probably require

several different programs. If sufficient storage is available it should be possible to put out only the parameters of the maximum and of the peak shape. This would be easier to do in the second and third cases. The first case, except for enormous storage facilities, would require human selection of points to be used in defining the peak. These could then be fed back into the computer to determine peak parameters.

The use of the various techniques above would require several different programs, some of which are but poorly adapted to evaluation of the basic I.B.M. 650 machine. The advent of faster and larger computational machinery on campus will make most of the above techniques feasible. The following is a discussion of the programs which were written for the I.B.M. 650 as a start toward meeting the above needs.

2. Three dimensional block program

The first attempt to write an I.B.M. 650 program was to carry out the direct summation of series (4) over the basic 1/64 of the unit cell and then to expand to obtain the remainder of the unit cell. It was felt that the avoidance of the large quantities of intermediate data required by successive one dimensional summations would make up the difference in the efficiency of the approach. As mentioned before, the time required is, for series (4), directly proportional to the number of terms considered, while the time required

by the one dimensional summations is somewhat independent of the number of terms provided the number of terms is much less than the number of mesh points to be evaluated. Consequently, there must be some point at which the latter method becomes superior. This point was not an easy thing to decide in advance. The actual programming of the direct evaluation led to the conclusion that even for large two dimensional projections the latter method is superior, at least on the basic I.B.M. 650. This latter method subsequently found realization in the T.D.F. 40-80 program which will be discussed in the next section.

One of the things which had promoted so much interest in the direct method was the invention of a subroutine that could obtain, and store for future use, values of cos $\theta(hk\ell)$ or sin $\theta(hk\ell)$ evaluated along a line in the mesh. The time required, aside from initialization for the specific line, was one revolution of the drum per point in the line. This subroutine was so fast that it was hoped that the calculation by this method would make direct evaluation feasible. The use of the unexpanded form (4) is not feasible in general as was discussed above. However, if the number of terms involved or if the number of points involved are small, this procedure has many advantages, including that of speed. Consequently the unexpanded form is good for the evaluation of the electron density about a single maximum. Since, as was discussed, the three dimensional block evaluation is a

very useful tool it was decided to write such a program. To save more time, it was decided to open up the interior loops and write them out explicitly. Because of the increased initialization, this did not turn out to be a very good idea, and if the program were to be rewritten, this should not be done. Even so, the final program is quite satisfactory.

The overall design of the program having been carried out, the program was written in collaboration with Mrs. Phyllis A. Keys.

Since there is no need for expansion to other parts of the unit cell in such a program, subseries sums are not required. The summation is by a direct three dimensional procedure and so one pass of the coefficient cards produces a small set of output cards containing the values of the electron density. The values obtained are on the mesh points of a cube of 4 points to a side, that is, a total of 64 points. The mesh points are at such a spacing that there are 80 mesh points along each side of the unit cell. It was felt that this would be enough to define the peaks except possibly for very large cells. If the program were rewritten with uncut loops, it may be that more points could be accommodated. The program computes at a rate of approximately twenty reflections per minute. For a detailed description of the program and a set of operating instructions, please refer to Appendix A.

3. Block peak program

In accordance with the general discussion, it was felt that a program which could take the results of the three dimensional block program and generate a set of parameters describing the peak would be desirable. The procedure is to fit the electron density near the center of a peak using the function

$$\rho = \exp\left[a_0 + a_1x^2 + a_2y^2 + a_3z^2 + a_4x + a_5y + a_6z + a_7yz + a_8xz + a_9xy\right]$$

by means of a least squares treatment. This program was written by Mr. Donald E. Williams and is included here only to complete the discussion of this type of approach. The program was written in the Bell Laboratories interpretive routine and is quite rapid. About one minute is required for each peak. This program has been written up and is available from Mr. Williams (16). This program and the preceding block program are very useful during a refinement of a structure.

4. The T.D.F. 40-80 program

If the model is not firmly established, a complete search of the unit cell is needed. This may be accomplished either by rough scanning and using the block program about maxima or by evaluation of all points on a fine mesh. It

was found possible to write a program that could do either job. A mesh of 40 x 40 x 40 points is used for rough scanning and a mesh of 80 x 80 x 80 points is used when all points and a fine mesh are desired. The procedure is based on series (5).

The method of calculation is quite simple and involves the use of two trigonometric tables containing cos $2\pi hx$ and sin $2\pi hx$ for $h = 1,2,\ldots,39$ and $80\,x = 1,2,\ldots,19$. These values correspond to the 80 mesh program. They are reduced appropriately for the 40 mesh program. The functions are stored with rounded six significant figure accuracy. These tables occupy most of the drum storage. The special values not included above are computed by the program.

A one dimensional summation is evaluated for each pass of the cards. The output cards are then sorted and passed through the I.B.M. 650 again for the next sum. The time required for the calculation may be estimated from a card reading rate of approximately 100 cards per minute and a card punching rate of 100 cards per minute for an evaluation on the 80 x 80 x 80 mesh. The last summation punches results with ten points per card. The intermediate sums punch only one point per card. The number of subsums required depends upon the expansions required to cover that portion of the unit cell which is of interest. The card reading rate is much faster for the 40 x 40 x 40 mesh and, of course, the output from each summation is only half that of the

output from the 80 x 80 x 80 mesh evaluation. The output punching rate is still 100 cards per minute. The two programs can be mixed to give differing meshes in different directions. This calculation rate is close to the maximum rate at which cards can be read and punched. The calculations are carried out over only 1/4 x 1/4 x 1/4 of the unit cell. The remainder of the cell is obtained by combining the subsums appropriately at the same time the results are printed.

The time required for a calculation by the above method is essentially just that required to read and punch cards at a rate of 100 cards per minute. Any possible increase in speed as a result of reprogramming must come about through a reduction in the number of cards punched and read. It should be noted that the time being referred to is the time on the I.B.M. 650. Some time is required for sorting, but the expense of this is minor. After the T.D.F. 40-80 program was completed, a modification was discovered which effectively reduces the number of cards punched by a factor of from two to eight. This would now bring computation speeds up to a limit set by punching and reading times with actual internal calculations requiring only a minor amount of time. A further advantage of this modification is that sorting is eliminated for two dimensional evaluations and is greatly reduced for three dimensional evaluations. This modification will be made in the near future. Where an I.B.M. 650 with

magnetic tape attachment is available, the speed will be increased by a large factor by using this modification. For details of the T.D.F. 40-80 program please refer to Appendix B.

B. Least Squares Method

1. General problem

A least squares method was first applied to the refinement of crystal structures by E. W. Hughes (17). In order to make clear the application of computer methods and the usefulness of the least squares method, a detailed analysis of the method is given below.

The structure factor can be related to the parameters of the atoms in the crystal by

$$(7)\quad F(hk\ell)=\sum_i f_i(hk\ell)\,\exp\left[-B_i\,\sin^2\theta/\lambda^2\right]\exp 2\pi i(hx_i+ky_i+\ell z_i)$$

where λ = wave length of the radiation used,

θ = Bragg reflection angle,

B_i = isotropic temperature factor for atom i,

and x_i, y_i, z_i = coordinates of atom i expressed in fractions of the unit cell.

One measure of agreement between a trial model and the observed data is

$$(8) \qquad R_3 = \frac{\sum_u w_u \left(|F_o| - |F_{ct}|\right)^2}{\sum_u w_u |F_o|^2}$$

where u = index representing all $hk\ell$,

w_u = weighing factor for $u = h,k,\ell$,

$|F_o|$ = observed structure factor magnitude,

and $|F_{ct}|$ = calculated structure factor magnitude for the trial structure.

If the errors in the observed data obey a Gaussian distribution and if there are no errors in the calculation of F_{ct} the minimization of R_3 with respect to the parameters of the structure will lead to a most probable set of values for the parameters. A general discussion of this relationship is given by E. T. Whittaker and G. Robinson (18). If we denote the values of $|F_{ct}|$ based on the most probable structure by $|F_{cT}|$ we can expand $|F_{cT}|$ about $|F_{ct}|$ in a Taylor series and obtain

$$(9) \qquad |F_{cT}| = |F_{ct}| + \sum_{i=1}^{m} \Delta x_i F_i + \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \Delta x_j F_{ij} + \cdots$$

where m = total number of parameters,

Δx_i = corrections to be added to the parameters of the trial model,

$F_i = \left.\frac{\partial |F|}{\partial x_i}\right| x_i$ for the trial model,

$$F_{ij} = \frac{\partial^2 |F|}{\partial x_i \partial x_j} \Bigg|_{x_i}, \text{ for the trial model.}$$

The function R_3 will be a minimum when the trial structure is the most probable structure. This implies that

$$\frac{\partial}{\partial x_k} \left[\frac{\sum_u w_u (|F_o| - |F_{cT}|)^2}{\sum_u w_u |F_o|^2} \right] = 0 \tag{10}$$

By substituting the value of $|F_{cT}|$ from equation (9) into equation (10) we obtain a set of equations relating the Δx_i and the observed data. If the trial model is close enough to the most probable structure, we can neglect high order terms in the series (9) because of the smallness of the Δx_i. Retaining for the present all terms through the second order, we can write equation (10) after the substitution for $|F_{cT}|$ in the form

$$0 = \sum_u w_u \left[(|F_o| - |F_{ct}|)(-F_k) + \sum_{i=1}^{m} \Delta x_i F_i F_k \right.$$

$$- \sum_{i=1}^{m} \Delta x_i F_{ik} (|F_o| - |F_{ct}|)$$

$$\left. + \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \Delta x_j F_i F_{jk} \right]$$

$$+ \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \, \Delta x_j \, F_k \, F_{ij}$$

$$+ \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{\ell=1}^{m} \Delta x_i \, \Delta x_j \, \Delta x_\ell \, F_{ij} \, F_{\ell k} \Big] \, .$$

If we consider only the linear terms involving derivatives with respect to x_k, we can solve for the Δx_k to obtain

$$\Delta x_k = \frac{\sum_u w_u \left(|F_o| - |F_{ct}| \right) F_k}{\sum_u w_u \left[F_k^2 - F_{kk} \left(|F_o| - |F_{ct}| \right) \right]}$$

This last step is definitely an approximation and essentially corresponds to neglecting all terms of the Taylor series beyond the linear one. Only the second term in the denominator arises from the second order Taylor series term. The justification for using only linear terms is made on the grounds that the Δx_k are small and that the other terms tend strongly to cancel when summed. In any case, if the model is close enough the corrections will be valid. Because of the approximations involved, an iterative procedure is used by recalculating the F_{ct} for the new parameters and determining the new correction. The new corrections are usually too large and so, to prevent oscillation, they are reduced by a constant factor before the next cycle. It is possible to include many of the other terms, but this requires much more calculation. Several

cycles of the linear approximation could be computed in the time it would take to compute more accurate corrections. Convergence, if it occurs, is usually rapid enough to make the linear approximation quite satisfactory. There is good reason to think that one might get convergence from a poorer model if more of the cross derivatives were included. This is difficult, but not impossible to do using the I.B.M. 650.

The second term in the denominator is usually neglected also. This may not be a good approximation in some cases. Since this term is quite easy to include, it would probably be worthwhile to include it. The size of this correction may be judged from the ratio of one term in the denominator to F_k^2. This ratio is, if a center of symmetry is assumed,

$$1 - \frac{|F_{ct}|}{F_{ct}} (|F_o| - |F_{ct}|) \frac{\partial^2 F}{\partial x_k^2} \left(\frac{\partial F}{\partial x_k} \right)^{-2} \Bigg|_{x_k \text{ for the trial model}}$$

For the atomic position parameter of the r atom in the space group $P\bar{1}$ this ratio becomes

$$1 + (|F_o| - |F_{ct}|) \frac{|F_{ct}| \cos 2\pi(hx_r+ky_r+\ell z_r)}{F_{ct} f_r \exp\left[-B_r \frac{\sin^2\theta}{\lambda^2} \right] \sin^2 2\pi(hx_r+ky_r+\ell z_r)}$$

where x_r, y_r and z_r are the coordinates of the r atom in fractions of the unit cell dimensions. Because of alterations

of sign of the second term, the sum of such terms will tend to cancel. For the temperature factor of the r atom using the same space group the ratio becomes

$$1 - (|F_o| - |F_{ct}|) \frac{|F_{ct}|}{F_{ct}} \frac{\sin^2\theta}{\lambda^2} \left(\frac{\partial F}{\partial B_r}\right)^{-1}$$

Again such terms tend to cancel. In the early states of refinement, however, these differences tend to be systematic in sign and will then not cancel. It would appear that the inclusion of this term, particularly for temperature factor corrections, would be advisable.

The standard deviation of the parameters so obtained may be estimated (18) from the equation $\sigma^2(x_r) = \frac{\sigma^2}{D} B_{rr}$

where $\sigma^2 = \frac{\sum_u w_u (|F_o| - |F_{ct}|)^2}{u - m}$

u = total number of reflections,

m = total number of parameters being varied,

B_{rr} = r'th principle minor of D,

$$D = \begin{vmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{12} & b_{22} & \cdots & b_{2m} \\ \cdot & \cdot & \cdots & \cdot \\ b_{1m} & & \cdots & b_{mm} \end{vmatrix} ,$$

$$b_{ij} = \sum_u w_u \left[F_i F_j - \delta_{ij} (|F_o| - |F_{ct}|) F_{ij}\right] .$$

If b_{rj} $(j \neq r) \ll b_{rr}$, which will be the case if the peaks are well separated in an orthogonal cell,

$$\frac{B_{rr}}{D} = \frac{1}{b_{rr}}$$

and so

$$\sigma^2(x_r) = \frac{\sum_u w_u \left(|F_o| - |F_{ct}|\right)^2}{(u-m) \sum_u w_u \left[F_r^2 - \delta_{ir} \left(|F_o| - |F_{ct}|\right) F_{ir}\right]}$$

Since the values of $\sigma^2(x_r)$ have real meaning only when the refinement is completed, the term $\delta_{ir} \left(|F_o| - |F_{ct}|\right) F_{ir}$ can be ignored as it must tend to vanish in the sum.

A very good least squares program, written by M. E. Senko and D. H. Templeton (12) is available and has been used for many of the calculations involved in the following structural investigations. A brief description of this program will be given in the next section. The purpose of this description is to place in context the modifications discussed in the L.S.II M program.

2. L.S.II program

In the Senko-Templeton L.S.II program (12), the corrections to the parameters are computed by neglecting all second order terms in the Taylor series expansion and by neglecting all first order cross terms except those between x and z for the same atom and those between the temperature factor of the

first atom and the scale factor. The standard deviations are computed in a corresponding manner.

The structure factor and its derivatives are computed only for orthorhombic space groups. This subroutine can be rewritten for other space groups. In orthorhombic systems, the trigonometric part of the structure factor takes for its A part one of the forms

$$\cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z$$
$$-\cos 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \cos 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$

and for its B part one of the forms,

$$\sin 2\pi hx \cos 2\pi ky \cos 2\pi \ell z$$
$$\cos 2\pi hx \sin 2\pi ky \cos 2\pi \ell z$$
$$\cos 2\pi hx \cos 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$

where $F(hk\ell) = A + iB$. The form to be used is specified by appropriate codes on each reflection card. These forms, of course, must be multiplied by multiplicity factors, temperature factor corrections, and scattering factors to form the structure factor.

3. L.S.II M program

Because of the frequent occurrence of other crystal classes, a somewhat more flexible structure factor section was desired. This flexibility can be achieved by summing an arbitrary number of the various orthorhombic forms. If, in addition, the indices can be changed and more sets of sums added to the first set the program is suitable for essentially all space groups. The modifications to the L.S.II program are designed to accomplish this flexibility.

The structure factor and derivative subroutines are modified so as to accumulate results in work cells rather than only storing them in the work cells. An added routine, just before the make up of the arguments section will zero the work cells. Thus, for any one atom, the calculations are started with zero in each work cell. The subroutine exits have been so modified that after a B part has been obtained the corresponding A part is obtained and then the program refers to address 1999 of the magnetic drum storage of the I.B.M. 650. If two or more orthorhombic type terms are desired for the same indices, the A type subroutine exits are modified so as to refer to the entrance of the next desired term. The results are automatically accumulated. The program will, in any case, finally exit at 1999. At this point, an index modification routine may be inserted, and the program is then returned to the make up of arguments routine for the calculation of the next set of terms which are also automatically

summed with the previous results. This can be repeated as many times as is required. When the final structure factor and its derivatives are obtained, the modified program exits into the normal program. This requires the use of control cards which will couple the orthorhombic type routines as desired. If index modifications are required a short subroutine must be written and inserted at 1999.

There are a few other minor modifications to the L.S.II program which expand its usefulness. For details please refer to Appendix C.

III. STRUCTURAL DETERMINATIONS

A. Structure of $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

1. Data

Preliminary X-ray diffraction photographs using the Weissenberg and precession cameras verified the assignment by J. A. A. Ketelaar (10) of the space group C_{6h}^2 - $P6_3/m$. The only systematically missing reflections were of the type (00ℓ) with $\ell = 2n + 1$. Photographs taken with long exposure times indicated that the missing (00ℓ) reflections could not have an intensity above the background level. This would indicate that the true space group is probably either C_6^6 - $P6_3$ or C_{6h}^2 - $P6_3/m$, since general positions in the space group must be occupied. The structure was refined on the basis of the centrosymmetric space group C_{6h}^2 - $P6_3/m$. The excellent final results further confirm this symmetry.

A small crystal was mounted in such a way as to record the (h0ℓ) reflections on a back reflection Weissenberg camera. Measurement of the positions of these reflections at large angle gives lattice constants of $a = b = 13.915 \pm 0.001$ Å and $c = 7.064 \pm 0.002$ Å. The lattice constants reported by J. A. A. Ketelaar (10) are not quite as accurate, but the above values are within his limits of error. From the density of 1.96 (10) the number of formula weights per unit cell is found to be two.

The photographs to be used for intensity measurements were obtained using an approximately cylindrical crystal 0.5 mm in length and 0.1 mm in diameter. The axis of the cylinder was the crystallographic c-axis. The crystal was coated with a thin layer of Canada balsam to prevent loss of water. Molybdenum K_α radiation was obtained by filtering the radiation from a molybdenum X-ray tube through zirconium foil. Data were obtained, using this K_α radiation, by rotating the crystal about the c-axis in a Weissenberg camera and recording each layer line so produced. A total of nine layers, including the zero layer, were recorded. Two sets of standards spots were obtained. The spots used for the standard sets were taken from the zero and third layers. By judging the intensities of a given layer against that set of standard spots which had the same size and shape, it was possible in large measure to compensate for the variations of spot shape. Several film packs, with six films per pack, were exposed for varying times for each layer so that the intensities would overlap. The film transmission factor of Eastman Kodak X-ray film for molybdenum is 0.736. Each spot was judged on each film as long as it was in the range of the standard spots. By use of the film factor, all intensities were scaled up to the first, most intense, film and averaged. The average was taken using weights related to the reproducibility of measurement in the different parts of the standard spot range.

A standard judging procedure was set up and the actual intensity judgements were made by Mrs. Jean Kestel. Mrs. Kestel was unfamiliar with this work and was quite free of any bias in judging. After a very brief instruction period she was able to do an excellent job of judging the intensities. As she did not know the transmission factor of the film, each measurement of one reflection was quite independent of the others. To save confusion, the reflections were indexed by an overlying grid of lines on tracing plastic. One set of lines was numbered and each line corresponded to reflections having a common h value. The intersecting lines were lettered and each line corresponded to reflections having a common h + k value. This procedure gives a grid with each line crossing the others with a large angle of intersection, an aid in preventing mistakes. If the grid were the regular Weissenberg net, the intersections could occur at small angles with resulting uncertainties. The actual ($hk\ell$) indices were assigned from a knowledge of the letter and number assigned to the reflection by the grid. Each reflection was judged on as many films as possible. The data were then checked, indices assigned, and weighted averages computed. This procedure worked out with complete satisfaction. Approximately 1300 reflections were judged in this manner.

The reflection intensities were corrected for Lorentz and polarization factors by means of the INCOR (19) program for the I.B.M. 650. The INCOR program also evaluates

$\sin^2\theta/\lambda^2$ and looks up the values of the atomic form factors from tables punched into cards. Atomic form factors for carbon and oxygen were obtained from the work of J. Berghuis et al. (20), that for sulfur has been computed by H. Viervol and O. Ogrim (21), and that for erbium was obtained from the work of Thomas and Umeda (22). The values of $F(hk\ell)$ so obtained are given in Appendix D.

2. Trial structure

The possible sets of equivalent positions in the space group $P6_3/m$ are given in the International Tables for X-ray crystallography (23) and are reproduced in Table 1. The coordinates are given in terms of fractions of the unit cell.

As there are only two molecules per unit cell (10), the two erbium atoms must be assigned to one of the two fold sets. The erbium scattering power is so great that if it were assigned to either set a or set b the layers for odd values of ℓ would be composed of comparatively weak reflections. As this is not the case, the erbium atoms must be assigned either to set c or to set d. These two sets differ only in the position of the origin of the unit cell, and so set c was selected.

A two dimensional electron density projection using the (hk0) data and the signs of the erbium structure factor contribution was computed by the use of the T.D.F. 40-80 program for the I.B.M. 650. Because of the sixfold symmetry,

Table 1. Equivalent positions for space group $P6_3/m$

Wyckoff notation and point symmetry		Co-ordinates of equivalent positions			Conditions limiting possible reflections
i	1	x,y,z;	$\bar{y},x-y,z$;	$y-x,\bar{x},z$;	$(00\ell):\ell=2n$
		$\bar{x},\bar{y},\bar{z}$;	$y,y-x,\bar{z}$;	$x-y,x,\bar{z}$;	
		$\bar{x},\bar{y},\frac{1}{2}+z$;	$y,y-x,\frac{1}{2}+z$;	$x-y,x,\frac{1}{2}+z$;	
		$x,y,\frac{1}{2}-z$;	$\bar{y},x-y,\frac{1}{2}-z$;	$y-x,\bar{x},\frac{1}{2}-z$.	
h	m	$x,y,\frac{1}{4}$;	$\bar{y},x-y,\frac{1}{4}$;	$y-x,\bar{x},\frac{1}{4}$;	
		$\bar{x},\bar{y},3/4$;	$y,y-x,3/4$;	$x-y,x,3/4$.	$(00\ell):\ell=2n$
g	$\bar{1}$	$\frac{1}{2},0,0$;	$0,\frac{1}{2},0$;	$\frac{1}{2},\frac{1}{2},0$;	$(hk\ell):\ell=2n$
		$\frac{1}{2},0,\frac{1}{2}$;	$0,\frac{1}{2},\frac{1}{2}$;	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	
f	3	$1/3,2/3,z$;	$2/3,1/3,\bar{z}$;		$(hk\ell)$: if $h-k=3n$ then $\ell=2n$
		$2/3,1/3,1/2+z$;	$1/3,2/3,1/2-z$.		
e	3	$0,0,z$;	$0,0,\bar{z}$;		$(hk\ell):\ell=2n$
		$0,0,\frac{1}{2}+z$;	$0,0,\frac{1}{2}-z$.		
d	$\bar{6}$	$2/3,1/3,1/4$;	$1/3,2/3,3/4$.		$(hk\ell)$: if $h-k=3n$ then $\ell=2n$
c	$\bar{6}$	$1/3,2/3,1/4$;	$2/3,1/3,3/4$.		
b	$\bar{3}$	$0,0,0$;	$0,0,1/2$.		$(hk\ell):\ell=2n$
a	$\bar{6}$	$0,0,1/4$;	$0,0,3/4$.		

for each reflection (hk0) there are five other equivalent reflections ($\bar{k}\bar{i}0$), ($ih0$), ($\bar{h}\bar{k}0$), ($ki0$), and ($\bar{i}\bar{h}0$) where $i = \bar{h} + \bar{k}$. Only the monoclinic symmetry could be used in reducing the number of required coefficients for the Fourier summation. Consequently the reflections (hk0), (ki0) and ($\bar{i}\bar{h}0$) must be separately included. The atoms in the unit cell were remarkably well resolved in this projection, and rough x and y parameters for all of the atoms except for the carbons and the hydrogens were obtained. There were indications of possible carbon positions, but the interpretation of them was somewhat ambiguous. The rough parameters so obtained are given in Table 2.

The z-parameters can not be obtained directly from the electron density projection. However, from a knowledge of reasonable atomic radii, it is possible to assign either one of two sets of z-parameters. These two sets are given in Table 2 where either the upper set or the lower set of values may be used. The sixfold water molecules and the sulfur atoms cannot have the same z-parameter as this would place the water and a sixfold sulfate oxygen too close together. From a knowledge of the sulfate ion structure, the z-parameter, relative to the sulfur, can be deduced. The further assumption that the twelvefold water molecules are hydrating the metal ion allows an estimate of their z-parameters to be made. There was no very convincing way to

Table 2. Rough parameters from electron density projection

Number of positions and point symmetry		Atom	Co-ordinates x	y	z
2	$\bar{6}$	Erbium	0.333	0.666	0.250
6	m	Sulfur	0.319	0.371	0.250 0.750
6	m	Sulfate Oxygen	0.247	0.418	0.250 0.750
6	m	Sulfate Oxygen	0.224	0.242	0.250 0.750
12	1	Sulfate Oxygen	0.381	0.390	0.069 0.569
6	m	Water Oxygen	0.337	0.490	0.750 0.250
12	1	Water Oxygen	0.215	0.550	0.562

distinguish the two models from the information given by the (hk0) data and atomic radii.

3. Refinement of the trial structure

The trigonometric part of the structure factor expression for one general set of atoms is given for $\ell = 2n$ by

$$4 \cos 2\pi\ell z \left[\cos 2\pi(hx+ky) + \cos 2\pi(ky+iy) + \cos 2\pi(ix+hy)\right]$$

and for $\ell = 2n + 1$ by

$$-4 \sin 2\pi \ell z \left[\sin 2\pi(hx+ky) + \sin 2\pi(kx+iy) + \sin 2\pi(ix+hy)\right],$$

where $i = \bar{h} + \bar{k}$. This form is not suitable for computation by the L.S.II M program. By expansion, the above forms can be written as,

for $\ell = 2n$,

$$\begin{aligned} 4 \big[&\cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z - \sin 2\pi hx \sin 2\pi ky \cos 2\pi \ell z \\ &+ \cos 2\pi kx \cos 2\pi iy \cos 2\pi \ell z - \sin 2\pi ky \sin 2\pi iy \cos 2\pi \ell z \\ &+ \cos 2\pi ix \cos 2\pi hy \cos 2\pi \ell z - \sin 2\pi ix \sin 2\pi hy \cos 2\pi \ell z \big] \end{aligned}$$

and for $\ell = 2n + 1$,

$$\begin{aligned} -4 \big[&\sin 2\pi hx \cos 2\pi ky \sin 2\pi \ell z + \cos 2\pi hx \sin 2\pi ky \sin 2\pi \ell z \\ &+ \sin 2\pi kx \cos 2\pi iy \sin 2\pi \ell z + \cos 2\pi kx \sin 2\pi iy \sin 2\pi \ell z \\ &+ \sin 2\pi ix \cos 2\pi hy \sin 2\pi \ell z + \cos 2\pi ix \sin 2\pi hy \sin 2\pi \ell z \big]. \end{aligned}$$

By the use of the L.S.II M program, this form can be evaluated and the proper derivatives can be obtained. For each pass through the structure factor and derivative section, one pair of the six terms is evaluated and their derivatives are obtained. The indices are then altered and the next pair is evaluated and summed with the first pair. A second index modification follows and then the third term is computed and summed. The indices are then restored to their original values and the regular L.S.II program is entered again. The work cells used above are reset just before the first

entrance to the structure factor routine for each atom. In this program, the multiplicity factor used is one for the general 12 fold set and proportionately less for special sets. This involves adding a factor of 1/6 to those available in the program.

A few cycles of refinement of the (hkl) data using the erbium and sulfur parameters of each of the two possible trial models clearly indicated that the correct structure is the one assigning a z-parameter of 0.750 to the sulfur set of atoms. This then forces the choice of the remaining z-parameters to be the lower ones of the pairs given in Table 2. It should be noted that large corrections to the erbium parameters were indicated. This is, of course, nonsense. The reason for this is that the positional derivatives of the erbium positions vanish identically. Because of the 1/3 and 2/3 in the parameters and because of the method used to obtain the sines and cosines, enough error is introduced to produce a correction which is the ratio of two error terms. This results in erratic and meaningless corrections to the parameters of the erbium atoms. This can be taken care of by simply resetting the erbium parameters before each cycle.

The refinement of the trial model obtained above was carried out by least squares cycles using the (hk0) data. The z-parameters were, of course, not refined by this procedure. A constant weighting factor was used and values of

$R_1 = 0.1198$ and of $R_2 = 0.0193$ were obtained. R_1 and R_2 are defined by

$$R_1 = \frac{\sum_u (|F_o| - |F_{ct}|)}{\sum_u |F_o|}$$

$$R_2 = \frac{\sum_u (|F_o| - |F_{ct}|)^2}{\sum_u |F_o|^2} \quad ,$$

and are a measure of the agreement between the model and the data. Because of the errors in measuring the data an agreement factor of $R_1 \sim 0.1$ implies very good agreement. The R factor alone, however, is not enough to justify a model since a few important reflections may be matched very poorly. This would indicate that changes must be made in the model. Such was not the case here.

A few signs of the F(hk0) were changed by the inclusion of the other atoms and so another electron density projection was obtained. The carbon positions were still ambiguous, but it was possible, from packing considerations, to assign approximate parameters. These parameters were $x = 0.186$, $y = 0.031$ and $z = 0.750$ for one sixfold set of carbons and $x = 0.287$, $y = 0.181$ and $z = 0.750$ for the other sixfold set of carbon atoms. The inclusion of these carbon parameters lead to a further refinement of the model by least squares. The agreement factors thus obtained were $R_1 = 0.0884$ and

Table 3. Results of two dimensional least squares refinement of $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	(Z)	σ_x	σ_y
Er	01	1.37	0.3333	0.6666	0.2500	-	-
S	02	2.34	0.3205	0.3725	0.7500	0.0008	0.0008
$O(SO_4)$	03	2.83	0.2489	0.4211	0.7500	0.0022	0.0022
$O(SO_4)$	04	2.55	0.2259	0.2357	0.7500	0.0022	0.0021
$O(SO_4)$	05	3.68	0.3828	0.3960	0.569	0.0013	0.0013
$O(H_2O)$	06	3.29	0.3494	0.4927	0.2500	0.0024	0.0025
$O(H_2O)$	07	2.45	0.2133	0.5463	0.562	0.0011	0.0011
$C(CH_3)$	08	3.09	0.1767	0.0524	0.7500	0.0034	0.0034
$C(CH_2)$	09	3.12	0.2744	0.1671	0.7500	0.0034	0.0034

R_2 = 0.0097 which indicate remarkable agreement with the data. The resulting parameters, with their standard deviations are given in Table 3.

The set number used in Table 3 is merely an identification number used to keep the cards and calculations consistent. B is the temperature factor.

It is interesting to note the manner in which the scale factors, the temperature factors, and the positional parameters converged using the least squares method. The starting

model was most accurate with respect to positional parameters. The initial scale factors were approximate but crude. The initial temperature factors were just guesses but were approximately correct. The positional parameters moved very little in the first stages of refinement while the scale factor was refining. The temperature factors invariably increased during this period. Then in the middle part of the refinement, after the scale factor settled down the parameters would adjust. The temperature factors would remain steady or continue to increase. Then in the last stages, the temperature factors would drop sharply to their final values. This seems to be a quite general behavior as a similar behavior has been noted in essentially all of the least squares calculations for this and other structures. From this behavior, the conclusion that faster convergence for the temperature factor would substantially speed up the overall convergence would appear to be valid. The behavior of the temperature factor indicates that the approximations used in computing temperature factor corrections are not very satisfactory when the error in the temperature factor is not very small. Because of the lack of oscillation in the temperature factor, the damping factor for the corrections is satisfactory. The linear diagonal term arising from the second order term of the Taylor series expansion is not used in the L.S.II program. The form of this term is such as possibly to account for the temperature factor behavior. It

would be interesting to include this term but this has not been done as yet.

A least squares refinement using all of the data, about 1600 reflections including unobserved intensities, was carried out. The temperature factors and parameters from the two dimensional refinement cycles were used for the first three dimensional cycle of refinement. Approximate scale factors for each layer were obtained by taking a small number of reflections from each layer and refining crude guesses while holding all other parameters fixed. This was a very fast operation and it saves possibly several complete cycles with the bulk of the data. These scale factors were then used for the first three dimensional cycle. Each three dimensional cycle required approximately nine hours time on the I.B.M. 650. Five such cycles were computed using constant weighting factors and the results are shown in Table 4 and Table 5. The agreement factors for the complete data are $R_1 = 0.1016$ and $R_2 = 0.0203$ and are quite satisfactory.

The observed data and the calculated structure factors based on the above structure are given in Appendix D.

The signs of F(hk0) obtained from the above structure were used to recalculate the electron density projection onto the (001) plane. The values of $F_{obs}(010)$, $F_{obs}(020)$, $F_{obs}(110)$, $F_{obs}(120)$ and $F_{obs}(210)$ could not be obtained from the films since they occurred at too small a reflection angle. Since these reflections are very insensitive to the

Table 4. Scale factors and R values for $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Layer (ℓ)	Scale factor	R_2	Layer (ℓ)	Scale factor	R_2
0	9.746	0.0109	5	10.394	0.0303
1	8.255	0.0238	6	11.876	0.0395
2	9.146	0.0122	7	13.564	0.0321
3	8.048	0.0197	8	13.92	0.0391
4	9.143	0.0168	all	-	0.0203

Table 5. Parameters for $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	Z	σ_x	σ_y	σ_z
Er	01	1.27	.3333	.6666	.2500	-	-	-
S	02	2.02	.3191	.3720	.7500	.0003	.0003	-
O	03	2.83	.2489	.4216	.7500	.0012	.0012	-
O	04	2.80	.2289	.2425	.7500	.0012	.0012	-
O	05	3.43	.3826	.3948	.5780	.0009	.0009	.0019
O	06	2.67	.3509	.4947	.2500	.0011	.0011	-
O	07	2.72	.2138	.5458	.4868	.0008	.0008	.0017
C	08	3.95	.1772	.0523	.7500	.0020	.0020	-
C	09	4.01	.2727	.1693	.7500	.0020	.0020	-

parameters, the calculated values of these reflections were used in the electron density projection. The F(000) term has been omitted and the electron density function was computed with an arbitrary scaling factor. The resulting projection is shown in Figure 1. It can be seen that good resolution is obtained and even the carbon peaks are clearly defined. This resolution, in the presence of the heavy erbium atoms, is much better than one previously would have thought possible.

B. Structure of $Y(C_2H_5SO_4)_3 \cdot 9H_2O$

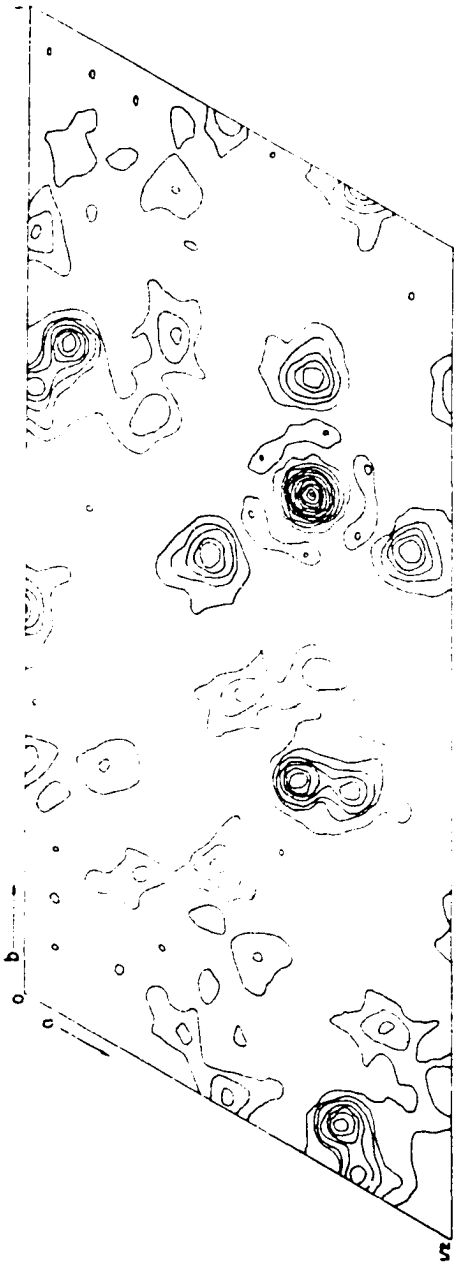
1. Data

The preliminary data again, and for the same reasons, indicated that the assignment of the C_{6h}^2 - $P6_3/m$ space group to this compound by J. A. A. Ketelaar (10) was correct. A precision determination of the lattice constants by a back reflection technique gave the values a = b = 13.9245 0.001 Å and c = 7.057 0.002 Å. This indicated that the $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ was isomorphous to the $Er(C_2H_5SO_4)_3 \cdot 9H_2O$ crystal.

Because of the fluorescence of yttrium in molybdenum K_α radiation, copper K_α radiation was used to obtain the intensity data. It was possible to obtain data using the Weissenberg camera for only five layers including the zero layer. Approximately 600 reflections were measured. The

Figure 1. The projection of the electron density of erbium ethylsulfate onto the (001) plane

The value of F(000) was omitted in this calculation and an arbitrary scaling factor was used. The contours are therefore in arbitrary units. The contours about the erbium atom are spaced at four times the value of the other contours.


b
0
0
5

judging procedure was the same as that used in the case of the erbium compound. The measured intensities were then corrected for the Lorentz and polarization factors by use of the INCOR program (19).

The intensities indicated that the only possible difference between the yttrium and erbium structures was one of small parameter shifts. Consequently, the parameters of the $Er(C_2H_5SO_4)_3 \cdot 9H_2O$ structure were used as the trial model for the yttrium compound. A projection of the electron density onto the (001) plane gave essentially the same results as for the erbium compound.

2. Refinement of the trial structure

In order to reduce the required number of three dimensional refinement cycles, the x and y parameters were refined using the (hk0) data only. Four cycles of least squares refinement using constant weighting factors were computed. The resulting parameters are given in Table 6. The agreement factors attained are $R_1 = 0.0913$ and $R_2 = 0.0125$.

There is reason to believe that the true weighting factors which should be used in a least squares refinement are not constant. The true weighting factors should be inversely proportional to the square of the probable error of the corresponding observed structure factor magnitude (18). Mr. Donald E. Williams (16) studied the measurement errors and concluded that it would be reasonable to assume that the

Table 6. Results of two dimensional least squares refinement of $Y(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	(Z)	σ_x	σ_y
Y	01	2.49	.3333	.6666	.2500	-	-
S	02	2.25	.3176	.3713	.7500	.0004	.0004
O	03	2.74	.2451	.4121	.7500	.0009	.0009
O	04	3.69	.2355	.2467	.7500	.0012	.0012
O	05	3.99	.3836	.3948	.5780	.0006	.0006
O	06	4.82	.3463	.4911	.2500	.0014	.0014
O	07	2.89	.2127	.5446	.4868	.0006	.0005
C	08	7.34	.1726	.0442	.7500	.0026	.0033
C	09	3.59	.2734	.1657	.7500	.0019	.0018

probable error in the observed structure factor magnitudes is given by the formulae

$$\Delta F_o = \frac{c}{200} F_o \quad \text{for} \quad I_o \geq 16\ I_m,$$

and

$$\Delta F_o = \frac{kF_m^2}{2F_o} \quad \text{for} \quad I_o < 16\ I_m,$$

where c = percentage error in observed intensities I_o,

kI_m = absolute error in I_o

I_m = background intensity

F_m = value of F corresponding to I_m.

To a first approximation, F_m^2 is a constant and so, in the second case above, ΔF_o is inversely proportional to F_o. The corresponding weighting factor expressions were programmed and inserted into the L.S.II M program. Any reference to variable weighting factors in the following discussion will mean the weighting factors based upon the above errors. It should be mentioned that, when variable weighting factors are used, a third R value, R_3, is obtained from the L.S.II and the L.S.II M programs. R_3 is defined by

$$R_3 = \frac{\sum_u w_u (|F_o| - |F_{ct}|)^2}{\sum_u w_u |F_o|^2}$$

and is an especially sensitive measure of agreement.

Least squares refinements using all of the data were carried out using both constant and variable weighting factors. Five cycles using constant weights were followed by two cycles using variable weights. Because of the previous constant weight refinement, the variable weight refinement converged in the two cycles. This does not indicate faster convergence with variable weights. The results of this refinement procedure are given in Table 7 and Table 8. The upper values in each table are the results of constant

Table 7. Scale factors and R values for $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ for refinement with constant (upper values) and variable (lower values) weighting factors

Layer	0	1	2	3	4	All
Scale Factor	2.024 1.997	2.143 2.175	2.325 2.295	1.838 1.751	1.661 2.153	- -
R_3	0.0048 0.0052	0.0041 0.0035	0.0048 0.0048	0.0076 0.0055	0.0119 0.0092	0.00607 0.00537
R_2	0.0089 -	0.0082 -	0.0099 -	0.0097 -	0.0245 -	0.0102 0.0117
R_1	- -	- -	- -	- -	- -	0.0808 0.0881

weighting factors and the lower values are the results for variable weighting factors. The R_3 values for constant weights were obtained from the next, variable weight cycle.

It can be seen that the use of variable weighting factors did not affect the R factors very much but that there was some change in scale factors. The large change in the scale factor for the fourth layer is probably due to the preponderance of weak reflections in that layer.

The temperature factors for the light elements are somewhat dependent upon the weighting factors used. This should sound a note of warning about the use of anisotropic temperature factors. Anisotropic factors should be even more

Table 8. Parameters for $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ for constant (upper values) and variable (lower values) weighting factors

Atom	Set number	B	X	Y	Z	σ_x	σ_y	σ_z
Y	01	2.47	.3333	.6666	.2500	-	-	-
		2.65	.3333	.6666	.2500	-	-	-
S	02	2.58	.3187	.3715	.7500	.0003	.0003	-
		2.34	.3195	.3715	.7500	.0005	.0005	-
O	03	3.85	.2485	.4205	.7500	.0009	.0009	-
		4.29	.2482	.4188	.7500	.0013	.0013	-
O	04	3.97	.2298	.2443	.7500	.0009	.0009	-
		4.47	.2305	.2446	.7500	.0014	.0014	-
O	05	3.95	.3837	.3947	.5763	.0006	.0006	.0014
		4.28	.3833	.3940	.5759	.0008	.0009	.0015
O	06	3.01	.3525	.4936	.2500	.0008	.0008	-
		3.11	.3524	.4920	.2500	.0011	.0013	-
O	07	3.17	.2122	.5452	.4854	.0005	.0005	.0014
		3.26	.2129	.5462	.4873	.0008	.0008	.0021
C	08	5.76	.1793	.0515	.7500	.0017	.0017	-
		6.71	.1815	.0526	.7500	.0023	.0023	-
C	09	4.63	.2751	.1650	.7500	.0015	.0015	-
		5.74	.2755	.1655	.7500	.0025	.0025	-

sensitive to systematic errors in the data. The use of such factors should be valid only if all systematic errors in the data and calculations are properly accounted for. This is obviously not true for these data. However, the differences in the temperature factors above should give a good measure of the accuracy to be expected in the isotropic temperature factors.

Fortunately, it appears that the weighting factors have little effect on the positional parameters. The largest difference, aside from the carbon parameters, amounts to only 0.02 Å in the parameter. One carbon parameter changed by 0.03 Å. These changes are of the same order as the standard deviations in the parameters.

The observed data and the calculated structure factors are given in Appendix D.

C. Structure of $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$

1. Data

Preliminary photographs verified that the praseodymium compound is isomorphous with the erbium and yttrium compounds. Because there was interest in the symmetry of the water molecules about the rare earth ion and because small differences from the erbium compound might not affect the intensities very much, partial data was obtained and analyzed. Precision cell constants were not measured. The cell

constants determined by J. A. A. Ketelaar (10) were used in this investigation. The cell constants are a = b = 14.035 Å and c = 7.104 Å.

The (hk0) data were obtained using a Weissenberg camera and molybdenum radiation. The intensities were judged in the same manner as for the erbium and yttrium compounds. The intensities were corrected for Lorentz and polarization factors by the INCOR (19) program. Comparison of these intensities with the (hk0) intensities of erbium indicated a very close correlation. Consequently, the structure of the erbium compound should be a satisfactory trial model for the refinement of this structure. The data so obtained is given in Appendix D.

2. Refinement of the trial structure

Four cycles of L.S.II M refinement were enough to give convergence from the trial model. Constant weighting factors were used. The agreement factors were R_1 = 0.0951 and R_2 = 0.0157. The parameters obtained are given in Table 9.

The Y parameter for set 05 is chosen so as to give a consistent S - O distance and is 0.5770. The Y parameter for set 07 is estimated, from the increase in the size of the rare earth ion, to be 0.4947.

The high temperature factor, B, for set 05 is probably due to insufficient resolution of this set from the set of sulfur atoms. The shifts in the parameters are small enough

Table 9. Parameters of $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	σ_x	σ_y
Pr	01	1.03	.3333	.6666	-	-
S	02	1.81	.3178	.3710	.0008	.0008
O	03	2.79	.2476	.4207	.0024	.0024
O	04	2.92	.2292	.2422	.0025	.0025
O	05	3.67	.3819	.3958	.0014	.0014
O	06	3.03	.3570	.4908	.0026	.0025
O	07	2.90	.2081	.5418	.0012	.0013
C	08	3.60	.1786	.0566	.0041	.0040
C	09	4.13	.2763	.1748	.0044	.0044

to indicate that there is little difference between the praseodymium and erbium compounds except for the size of the rare earth ion.

D. Discussion of Structures

1. Coordination of the rare earth ion

The structures of the erbium, yttrium and praseodymium ethylsulfates are essentially identical within experimental

error, the sole difference being one of ionic size. The general features of this structure are shown in Figure 2.

The rare earth ion is surrounded by nine water oxygens with the symmetry C_{3h}. Six water oxygens are placed above and below the rare earth ion at the six corners of a triangular prism. The remaining three water oxygens are placed out from the three vertical faces of the prism in the same plane as the rare earth ion. These three water oxygens are farther away from the rare earth ion than are the six above and below the rare earth ion. The metal to water oxygen distances are given in Table 10. These distances were calculated by the use of the distance program (25) for the I.B.M. 650. The symmetry of this arrangement could be D_{3h} but there is a slight rotation of the water oxygens, in the plane of the rare earth ion, with respect to the six water oxygens out of the plane. A rotation of the water oxygens in the plane of 4°23', 5°5', and 6°25' for the erbium, yttrium and praseodymium compounds respectively would restore the D_{3h} symmetry. The possible positions of the hydrogen atoms will be discussed in a latter section.

The ethylsulfate oxygens are arranged about the rare earth ion with C_{3h} symmetry as shown in Figure 2. There are a total of 18 ethylsulfate oxygens as next nearest neighbors about the rare earth ion. The distances from the rare earth ion are given in Table 10. The ethyl groups are packed closely about origin of the unit cell. This packing about

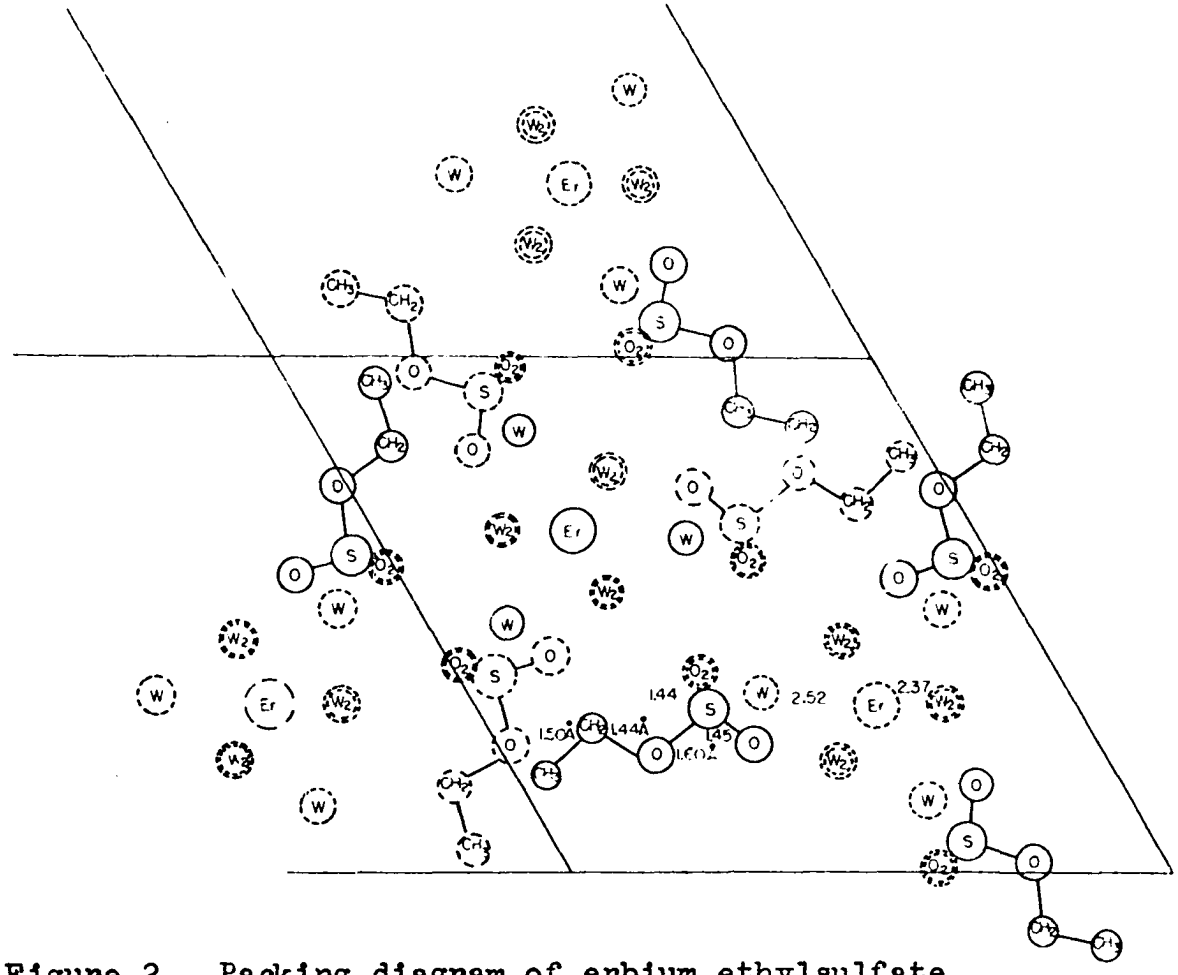


Figure 2. Packing diagram of erbium ethylsulfate

The solid circles represent atoms in the plane z = 1/4.

Table 10. Distances from the rare earth ion in Å

Atom	Set number	Quantity	Distance from Er	Distance from Y	Distance from Pr
$O(H_2O)$	06	3	2.52	2.55	2.65
$O(H_2O)$	07	6	2.37	2.37	2.47[a]
$O(-SO_4)$	03	6	4.63	4.64	4.65
$O(-SO_4)$	05	6	4.77	4.77	4.77[a]
		6	4.61	4.60	4.66[a]
$S(-SO_4)$	02	3	5.13	5.13	5.18
		6	5.33	5.34	5.36
$O(C_2H_5O-)$	04	3	5.56	5.57	5.61

[a]The calculation of these distances requires Y parameters which have been estimated from the structure of the ethylsulfate ion and from the increase in the radius of the rare earth ion.

the 6_3 axis at the origin leads to infinite cylinders of hydrocarbon material at the origin of the unit cell.

The hydrogens attached to the carbon atoms can be placed so as to preserve the C_{3h} symmetry. This requires that one of the methyl hydrogens lies in the mirror plane. The packing, with such an arrangement, is quite reasonable. There is no reason to suppose that the hydrogens violate the C_{3h} symmetry.

2. The ethylsulfate ion structure

The structure of the ethylsulfate ion has been determined during a structural investigation of potassium ethylsulfate by J. A. J. Jarvis (24) using three dimensional Fourier techniques. The distances within the ethylsulfate group are shown in Table 11. The distances for the potassium compound are also given.

Table 11. Ethylsulfate ion distances in Å

From set	To set	Distance Er	Y	Pr	K
02-S	03-0	1.45	1.45	1.46	1.49
02-S	05-0	1.44	1.46	1.45	1.44
02-S	05-0	1.44	1.46	1.45	1.45
02-S	04-0	1.60	1.57	1.60	1.60
04-0	09-C	1.44	1.52	1.40	1.44
09-C	08-C	1.50	1.47	1.54	1.51
04-0	05-0	2.45	2.45	2.47	2.46
04-0	05-0	2.45	2.45	2.47	2.44
04-0	05-0	2.37	2.33	2.39	2.41
03-0	05-0	2.40	2.42	2.41	2.43
03-0	05-0	2.40	2.42	2.41	2.30
05-0	05-0	2.43	2.45	2.44	2.36

Considering the comparatively large atomic numbers of Er and Y, the agreement with the potassium ethylsulfate results is remarkable. The spread in the equivalent S-O distances is only 0.01 Å for the heavy metal compounds. The O-C-C distances are in good agreement, although it would appear that the O9-C set for yttrium ethylsulfate has not refined as well as in the other cases. The temperature factor for this carbon is a little smaller than for the others. The differences in position are small enough to be explained by the combination of an error in the position of the O4-O set of approximately 0.03 Å with an error in the opposite direction of 0.05 Å in the position of the O9-C set. This is about the same size as the standard deviation in the positions. It should be noted, however, that with this one exception the bond lengths are self consistent with an accuracy much better than would be required by the standard deviations.

3. The position of hydrogen bonds

The actual positions of the hydrogen atoms has not, of course, been determined. The positions of hydrogen bonds can be deduced in some cases from a knowledge of the interatomic distances of the atoms which could be attached to a hydrogen. These distances are given in Table 12.

The interpretation of these distances in terms of hydrogen bonds is obviously not unambiguous. However, if there

Table 12. Oxygen-oxygen distances

From water oxygen	To atom	Set number	Number of distances	Distance Er	Y	Pr
06	Sulfate Oxygen	05	2[a]	2.85	2.83	2.77[b]
	Water Oxygen	07	2	2.88	2.91	3.07[b]
	Water Oxygen	07	2	2.68	2.68	2.76[b]
07	Sulfate Oxygen	03	1[a]	2.74	2.76	2.76[b]
	Sulfate Oxygen	05	1[a]	2.85	2.81	2.83[b]
	Water Oxygen	06	1	2.88	2.91	3.07[b]
	Water Oxygen	06	1	2.68	2.68	2.76[b]
	Water Oxygen	07	2	2.89	2.92	3.04[b]

[a]Underlined atoms are thought to be hydrogen bonded.

[b]These values are obtained from estimated parameters.

were hydrogen bonding between the water molecules (sets 06 and 07) it would place the corresponding protons comparatively close to the metal ion and would orient the water dipole in opposition to the strong electric field between the metal ion and the sulfate oxygens. Hydrogen bonding between the

waters and the sulfate oxygens would place the protons much closer to the negative oxygens and would align the water dipoles with the electric field. The second possibility would seem to be more reasonable provided the oxygen positions produced the proper oxygen to oxygen distances and the resulting angles were reasonable. It can be seen in Table 12 that the required sulfate oxygen positions are present. The angle formed by the two set 05 oxygens with set 06 water oxygen of 107°39' is quite reasonable. The hydrogen bond distance of 2.85 is also reasonable. Hydrogen bonding in this manner could also explain the loss of D_{2h} symmetry of the water polyhedron and the longer water to metal ion distance for the set 06 oxygens. The hydrogen bonds are slightly long. This would indicate that the set 06 oxygens are balancing between the metal ion attraction and the hydrogen bond contraction. This would tend to rotate the 06 set with respect to the 07 set. This rotation would also tend to align the water dipole even more in the direction of the field. It is this rotation that is responsible for destroying the D_{3h} symmetry of the oxygen polyhedron about the metal ion.

The set 07 water oxygens can form hydrogen bonds to the set 03 and set 05 sulfate oxygens. The bonds are of unequal length, 2.74 Å and 2.85 Å, and the H-O-H angle is 94°37'. The water dipole is closely aligned with the electric field.

This hydrogen bond structure should, consequently, give the lowest energy.

It should be noted that any reasonable placement of hydrogen bonds must violate D_{3h} symmetry and produce C_{3h} symmetry.

4. The Jahn-Teller effect

As was expected from the work of J. H. VanVleck (8)(9), no Jahn-Teller distortion could be detected in the praseodymium salt. The distortions produced must be less than the experimental errors in the structure determination. Because of the excellent refinement of the (hk0) data, the threefold symmetry must be very closely obeyed.

It should be noted that the Jahn-Teller effect is not to be expected in the yttrium and erbium salts because of the occurrence of Kramers degeneracy. This is the only type of degeneracy present and no electric field can split the Kramers degeneracy. Distortions in such a case do not necessarily lead to lower energy for the molecule. An interesting derivation of Kramers degeneracy is given by J. M. Jauch (26) which clearly shows Kramers degeneracy to be independent of the field.

IV. SUMMARY

A. Computing Methods

A discussion of the various methods of evaluation of Fourier series was given. The use of the Fourier series in obtaining trial structures and in refining trial structures is discussed. These two uses require, for optimum results, different approaches. The T.D.F. 40-80 program for the I.B.M. 650 was written to satisfy the first of these needs and the T.D.F. 80 block program was written to satisfy the second of these needs.

A discussion of the least squares method as applied to refinement of crystal structures is given. A modification of the Senko-Templeton L.S.II program that will permit the use of more complex symmetry relationships in computing structure factors and in refining crystal structures has been made.

B. Structure Determination

The structures of erbium and yttrium ethylsulfate nonahydrate have been determined and refined by a three dimensional least squares method. The refinement produced R_1 values of 0.1016 for the erbium compound and of 0.0808 for the yttrium compounds for the three dimensional data. The

structure of the praseodymium compound was determined by a two dimensional refinement using a least squares method. The R_1 value for these data was 0.0951. The two Z parameters were not refined.

The structures of the rare earth ethylsulfates studied are isomorphous. The symmetry about the metal ion is C_{3h}. The water molecules are arranged about the metal ion in a polyhedron of C_{3h} symmetry. The symmetry of this polyhedron is approximately D_{3h}.

The possible positions of hydrogen bonds are also discussed.

V. BIBLIOGRAPHY

1. Sayer, E. V. and Freed, S. J. Chem. Phys. 24 1213 (1956).

2. Bleaney, B., Scovil, H. E. D., and Trenam, R. S. T. Proc. Roy. Soc. (London) 223A 15 (1954).

3. Bozorth, R. M. Bell Telephone Laboratories. Private Communication (1957).

4. Spedding, F. H. and Co-workers Ames Laboratory of the Atomic Energy Commission. Private Communication (1958).

5. Jahn, H. A. and Teller, E. Proc. Roy. Soc. (London) 161 220 (1937).

6. Jahn, H. A. Proc. Roy. Soc. (London) 164 117 (1937).

7. Kramers, H. A. Proc. Acad. Sci. Amst. 33 959 (1930).

8. VanVleck, J. H. J. Chem. Phys. 7 6 (1939).

9. VanVleck, J. H. J. Chem. Phys. 7 72 (1939).

10. Ketelaar, J. A. A. Physica 4 619 (1937).

11. International Business Machines Corporation. 650 Magnetic Drum Data-Processing Machine Manual of Operation. Rev. ed. The Corp. (1955).

12. Senko, M. E. and Templeton, D. H. University of California. Private Communication (1957).

13. Lipson, H. and Cochran, W. The Determination of Crystal Structures, Chapter 1. in Bragg, L., ed. The Crystalline State, Volume 3. London, G. Bell and Sons, Ltd. (1953).

14. Lipson, H. and Cochran, W. The Determination of Crystal Structures, Chapter 1. in Bragg, L., ed. The Crystalline State, Volume 3. London, G. Bell and Sons, Ltd. (1953).

15. James, R. W. The Optical Principles of the Diffraction of X-Rays, Chapter 2. in Bragg, L., ed. The Crystalline State, Volume 2. London, G. Bell and Sons, Ltd. (1954).

16. Williams, D. Ames Laboratory of the Atomic Energy Commission. Private Communication (1957).

17. Hughes, E. W. J. Am. Chem. Soc. 63 1737 (1941).

18. Whittaker, E. T. and Robinson, G. The Calculus of Observations, Chapter 8. London, Blackie and Son (1941).

19. Templeton, D. H. University of California. Private Communication (1957).

20. Berghuis, J., Haanappel, I. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendaal, A. L. Acta Cryst. 8 478 (1955).

21. Viervol, H. and Ogrim, O. Acta Cryst. 2 277 (1949).

22. Thomas, L. H. and Umeda, K. J. Chem. Phys. 26 293 (1957).

23. Henry, N. F. M. and Lonsdale, K. International Tables for X-Ray Crystallography, Volume 1. Birmingham, England. The Kynoch Press (1952).

24. Jarvis, J. A. J. Acta Cryst. 6 327 (1953).

25. Templeton, D. H. University of California. Private Communication (1957).

26. Jauch, J. M. U. S. Atomic Energy Commission Report, ORNL 813 (Oak Ridge National Laboratory Report). September 15, 1950. (Office of Technical Services, Washington 25, D. C.)

VI. ACKNOWLEDGMENTS

The author is deeply grateful to Dr. R. E. Rundle for his continued interest and support which made this investigation possible. The author is also indebted to Mr. D. E. Williams and Mrs. P. A. Keyes for their suggestions and assistance in writing some of the I.B.M. type 650 programs described in this work.

The author would like to thank Dr. F. H. Spedding for his interest and support of this research. The ethylsulfate compounds used in this investigation were prepared by B. C. Gerstein, R. V. Colvin, and J. R. Mullaly.

VII. APPENDIX A: T.D.F. 80 B PROGRAM

A. Fourier Series Evaluation for a 4x4x4 Point Block

1. Mathematical method

This program carries out the Fourier synthesis

$$\rho(x,y,z) = \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{\ell=0}^{\infty} |F(hk\ell)| \cos 2\pi(hx+ky+\ell z \pm \alpha)$$

in three dimensions within the unit cell on lattice points formed by subdivision of the unit cell at intervals of 1/80th. The series is evaluated for an arbitrary 4x4x4 point block. $F(hk\ell)$ is the structure factor and α is the phase angle, expressed as an integral multiple of 1/80th. The quantity actually entered into the 650 is α' where $\alpha' = n/80$ (4000) and $n = 0,1,2,\ldots,79$. The first four sections of the program locate and store the necessary cosines from three cosine decks located at optimum intervals on the drum. The breakdown of the program into sections is indicated in the flow diagram, Figure 3. Each cosine deck occupies two full lines (80 storages) across the drum, with the first line running from zero to $39/40\pi$ and the second from π to $79/40\pi$. Cosines are located by systematically altering the data address of a "load distributor" order which is carried in the upper accumulator; the variable instruction address of this order

refers to a "store distributor" order.

Each block is entered with the point (x_o,y_o,z_o) which is the "origin point". The program then systematically raisss these coordinates to (x_o,y_o+3,z_o+3) for the first plane, after which x_o is raised to (x_o+1) etc. to compute four planes of sixteen points each, or a total or sixty-four points for the block.

The four cosine sections compute the functions

$$\cos 2\pi(hx + ky + \ell z \pm \alpha),$$
$$\cos 2\pi(-hx - ky + \ell z \pm \alpha),$$
$$\cos 2\pi(hx - ky + \ell z \pm \alpha),$$
$$\cos 2\pi(-hx + ky + \ell z \pm \alpha).$$

This feature permits greater speed, if the crystal possesses symmetry such that $F(hk\ell)$ is the same for two or more of these permutations; in such cases, the cosines are summed algebraically before multiplication, so that fewer lengthy multiplications need be done.

Section 5 carries out the algebraic summation of cosines (provision is made for altering the sign of the cosines in each permutation) and the multiplication by $F(hk\ell)$. This product is then added to the partial sum for the previous reflections and stored. In centrosymmetric cases, $F(hk\ell)$ rather than $|F(hk\ell)|$ can be used.

Section 6 contains the procedure, necessary at the end of each plane, for raising the x-coordinate for the cosine

blocks and altering various constants for section 5.

Section 7 is the routine referred to immediately after reading a detail card with new F, h, k, ℓ, and α'. It sets up the initial angles for sections 1-4 and initializes the constants necessary to pass from one point to the next higher within a line, and from one line to the next higher within a plane.

Section 8 modifies the orders which pick up cosines in section 5, inserting an "add lower" order if F(hkℓ) is to be added in a given permutation, "a subtract lower" if it is to be subtracted and a "no-op" if that permutation was not computed in a given problem. This section functions only upon reading of a special "modification card" (See "Detailed Operating Instructions") which gives the necessary orders to be entered for the ensuing class of reflections. Section 8 also inserts the proper signs for α', the phase angle, in each permutation; the orders for this purpose are read from a second modification card. This second card is omitted if $\alpha' = 0$.

Section 9 punches out the sixty-four final sums, on eight cards, after completion of the program. It is loaded only at the end of the program because of insufficient drum space, but the punch routine loads into erasable storage and does not affect the subsequent use of the main program for additional blocks. Section 9 must, however, be reloaded at the end of each new block. Each storage whose contents

are punched is cleared to zero. The routine computes and punches plane number and range for each output card.

2. Range and accuracy

This is a fixed-point routine; the output cards contain six digits of each final sum with the scale of the results shifted the same amount as the $F(hk\ell)$ if a scaling factor is introduced. The indices h and k may have values from -39 to +39, and ℓ from 0 to 39. x_o, y_o, and z_o run from 0 to 80.

3. Storage

The block program uses the entire two-thousand words of drum storage. Of these, about two-hundred are temporary storages which may be used between reflections.

4. Speed

The program computes, on the average, about twenty detail cards per minute.

5. Equipment specifications

The basic I.B.M. 650 is required, with two-thousand words of drum storage. No special attachments to the machine are used.

6. Error checks

Storage 0000 contains an order which stops the machine if any of the instructions were not loaded onto the drum. The routine contains no other built-in error checks; however

the procedure can be checked by running overlapping blocks if machine errors are suspected.

7. Input-output

The format of input and output cards is discussed in more detail under "Detailed Operating Instructions". Input consists of detail cards containing $F(hk\ell)$, h, k, ℓ, α', special load cards specifying origin of block, permutations to be computed, and signs for $|F(hk\ell)|$ and phase angles in the different permutations. These special cards are multiple-order load cards which are read into 1951-1958. The detail cards are entered by board wiring and cause the program to start at the instruction address of the console, which is the first order of section 7. The detail card format may also be used for the Least Squares II calculation.

Output consists of eight punched cards each of which has the eight final sums for half of one plane. Plane number and range are punched in each card, as is the origin of the block, x_o, y_o, z_o.

8. Symmetry provisions

The form of the expression actually calculated is

$$\rho_{(xyz)} = \sum_{\substack{hk\ell \\ 0}}^{\infty} |F'(hk\ell)| \Big[\pm \cos 2\pi [hx + ky + \ell z \pm \alpha(hk\ell)] \pm \cos 2\pi [-hx - ky + \ell z \pm \alpha(\bar{h}\bar{k}\ell)] \pm \cos 2\pi [hx - ky + \ell z \pm \alpha(h\bar{k}\ell)] \pm \cos 2\pi [-hx + ky + \ell z \pm \alpha(\bar{h}k\ell)] \Big]$$

where F' represents structure factors divided by the proper factors required to take into account the differing multiplicities of non-general reflections.

$\alpha(hk\ell)$ must be an integral multiple of 1/80. If desired $F(hk\ell)$ instead of $|F(hk\ell)|$ can be used with no change in the program in the case of a center of symmetry. The program handles h and k algebraically. It also calculates any one or all of the permutations. If the algebraic form of the expressions does not change, the + and - index terms may be computed without modification by actually computing for negative indices. Modification cards are inserted between groups of reflections when the form must be changed.

B. Detailed Operating Instructions

1. Detail cards

One detail card is punched for each reflection, in the form hh kk$\ell\ell$ ab00 00 0000 0000 00 000F FFFF 00 0000 0000 00 0000 $\alpha'\alpha'\alpha'\alpha'$ 00 0000 0000 00 0000 0000 00 0000 00c0 , where a = sign of h, b = sign of k and c = sign of $F(hk\ell)$.

α' is expressed as n/80 (4000) where n = 0,1,...,79 and $n = \frac{80\,\alpha}{2\pi}$. α = phase angle in radians and is so chosen as to give integral n.

At the beginning of program, the read band contains the following:

1951	00	0000	0000 ,
1952	00	00hh	0000 ,
1953	00	00kk	0000 ,
1954	00	00$\ell\ell$	0000 ,
1955	00	FFFF	F000 ,
1956	00	$\alpha'\alpha'\alpha'\alpha'$	0000 ,
1957-1960	00	0000	0000 .

2. Special information cards

Special information cards are load cards and should have a Y-punch in the column used to identify load cards.

a. Switch cards There may be one, two or three of these cards which tell the program which permutations to compute. They are single-order load cards of form:

69 1954 1953^{Y} 00 0000 0000 24 XXXX 8000^{Y} 00 0000 ZZZZ^{Y}

where XXXX is one of the program section 1, 2, or 3 exits. These exits are 0994, 0284 or 0800 respectively. ZZZZ is the address of the next permutation to be computed.

If next desired section is 2 ($-hx - ky + \ell z \pm \alpha$), then

ZZZZ = 0934.

If next desired section is 3 ($hx - ky + \ell z \pm \alpha$), then

ZZZZ = 0100.

If next desired section is 4 ($-hx + ky + \ell z \pm \alpha$), then

ZZZZ = 0318.

If next desired section is 5 (Sum. and Mult.), then

ZZZZ = 1301.

b. Origin card The origin card contains starting coordinates, x_o, y_o, z_o in units of 1/80th of the unit cell with instructions for storing them. This card has the form

69 1956 1952^{Y} 24 1460 1953^{Y} 69 1957 1954^{Y} 24 1234 1955^{Y}
69 1958 1226^{Y} 00 0000 00$X_o$$X_o^{Y}$ 00 0000 00$Y_o$$Y_o^{Y}$
00 0000 00$Z_o$$Z_o^{Y}$.

c. Modification cards The modification cards contain the desired pick-up orders for the summation routine with orders for storing them, and also pick-up orders for the phase angle. The operation codes are 15 or 16 except for the first permutation used, in the first modification card. The codes used here must be 65 or 66.

The first modification card has the form 00 0000 0079^{Y}
aa 0027 0081^{Y} bb 1027 1334^{Y} cc 1077 0484^{Y} dd 0077 0731^{Y}
00 0000 0000 00 0000 0000 00 0000 0000 , where aa, bb, cc, and dd are operation codes for the first, second, third and fourth permutations respectively.

The second modification card controls the sign of the α' term in the argument of the cosine. This card is used only when α' is not zero and has the form 00 0000 1432^{Y}
ee 1956 0182^{Y} bb 1956 1513^{Y} gg 1956 0867^{Y} 69 1956 1957^{Y}
hh 1956 0513^{Y} 24 0148 8000^{Y} 00 0000 0000 , where ee, bb, gg, and hh are operation codes for the first through the fourth permutations.

3. Program loading cards

These cards are placed in front of the program deck and are used to zero the magnetic drum and to load the loading routine. These cards must be kept in the order below.

Card 1 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 0000 8000  00 0000 8000
           Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 2 is

```
Y          Y          Y          Y          Y
69 1952 1953  00 0001 0000  24 0001 1954  69 1955 1956
           Y          Y          Y          Y
10 0001 8003  24 0002 1957  61 1958 8003  20 1999 0002  .
```

Card 3 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 0000 8000  01 0000 8000
           Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 4 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 1082 8000  70 1950 1418
           Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 5 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 1950 8000  69 1952 1951
           Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 6 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 1157 8000  69 1954 1953
           Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 7 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 1613 8000  69 1956 1955
          Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 8 is

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 1884 1082  69 1958 1957
          Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

The format of the four order load cards is

```
Y          Y          Y          Y          Y
24 XXXX 1645  XX XXXX XXXX  24 XXXX 1695  XX XXXX XXXX
          Y          Y          Y          Y
24 XXXX 1745  XX XXXX XXXX  24 XXXX 0985  XX XXXX XXXX  ,
```

where the X's correspond to addresses and orders to be loaded. A transfer from the four order loading routine is made by punching the I address of the last store order on the last card with 8000.

The punching routine is loaded by single order load cards of the form

```
Y          Y          Y          Y          Y
69 1954 1953  00 0000 0000  24 XXXX 8000  XX XXXX XXXX
          Y          Y          Y          Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

The exit from this loading procedure is accomplished by a load card punched with `Y  Y` `00 0000 0009` in the first field.

4. Output cards

Two cards are punched for each of four planes. The first such card, identified by a 1 in. col. 1, contains final sums for points in the first two lines of the plane. These are punched in order of increasing Z coordinate, in the following

format:

Cols.	
1	Range number (1 or 2, for 1st, 2nd half-plane),
2	Plane number,
3,4	x_o,
5,6	y_o,
7,8	z_o,
13-18	Sum for x_o, y_o, z_o,
19-24	Sum for x_o, y_o, $(z_o + 1)$,
25-30	Sum for x_o, y_o, $(z_o + 2)$,
31-36	Sum for x_o, y_o, $(z_o + 3)$,
37-42	Sum for x_o, $(y_o + 1)$, z_o,
43-48	Sum for x_o, $(y_o + 1)$, $z_o + 1$,
49-54	Sum for x_o, $(y_o + 1)$, $z_o + 2$,
55-60	Sum for x_o, $(y_o + 1)$, $z_o + 3$.

The second card of each plane has final sums for the last two lines of the plane also arranged with increasing z's.

5. Operating procedure

Console should be set to 70 1951 1418. Sense switches and programmed stop switch are set to "stop". First two cards are a drum-clear routine for use with this console setting. They clear the entire drum to minus zeroes before loading in the four-order program load cards. Origin card is placed directly behind the program desk, followed by the

switch cards, then the two modification cards associated with the first class of reflections to be computed. Each new class of reflections must have these two modification cards in front of its detail cards. The detail cards go in after the special cards; they should be sorted on ℓ because considerable time can be saved whenever ℓ does not change between cards. The punch program is behind the last detail card. When the block is completed the machine will return to the console to read new origin card etc., for the next block. If no additional cards are in the card reader, program will stop on "input-output".

6. Flow diagram, program cards, and wiring diagram

The flow diagram for the T.D.F. 80 B program is given in Figure 3. The wiring diagram is given in Figure 4. The program cards are listed in Table 13. The quantities listed are the addresses and the orders. These must be made up into four-order load cards. The punch routine orders are listed in Table 14. These form single order load cards.

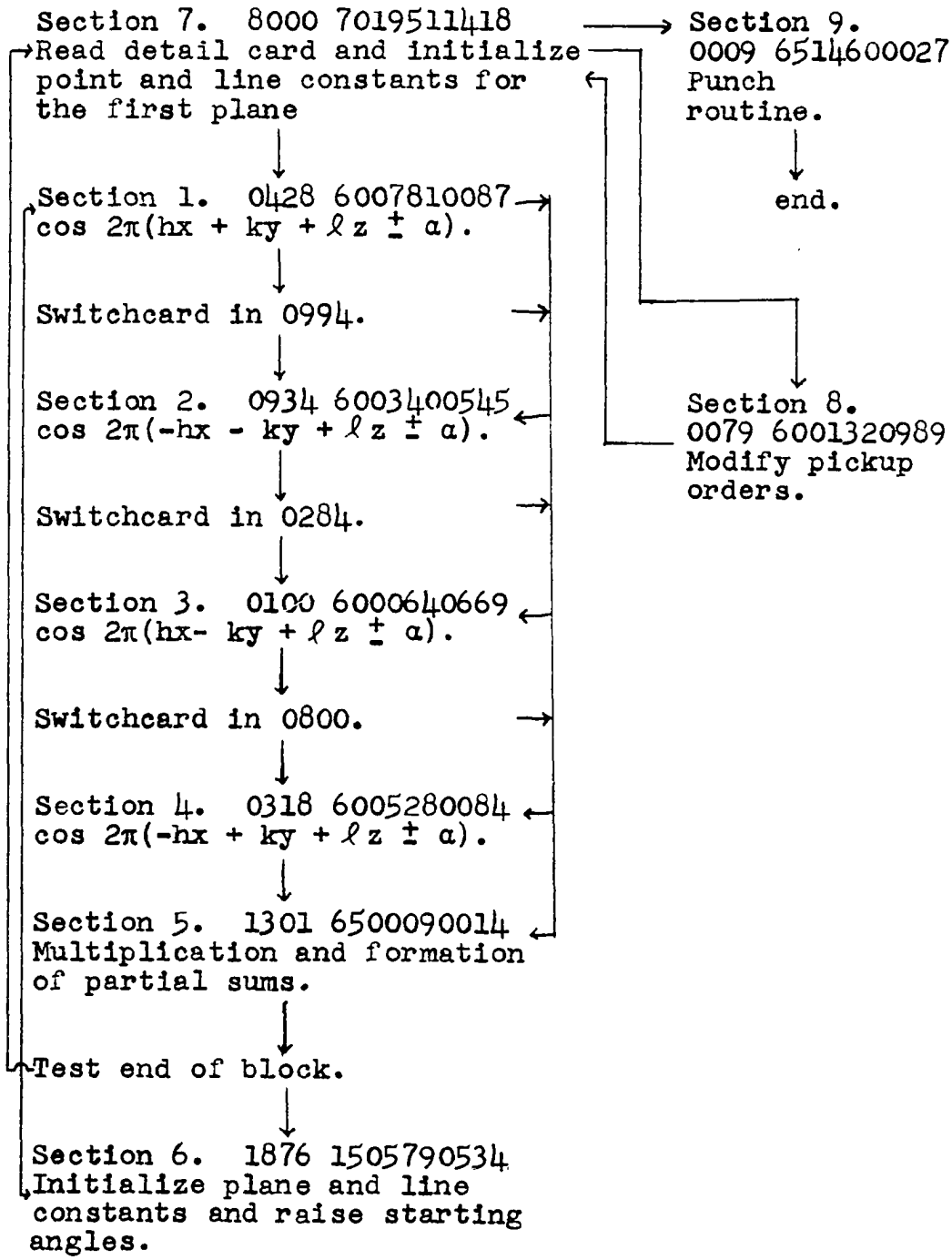
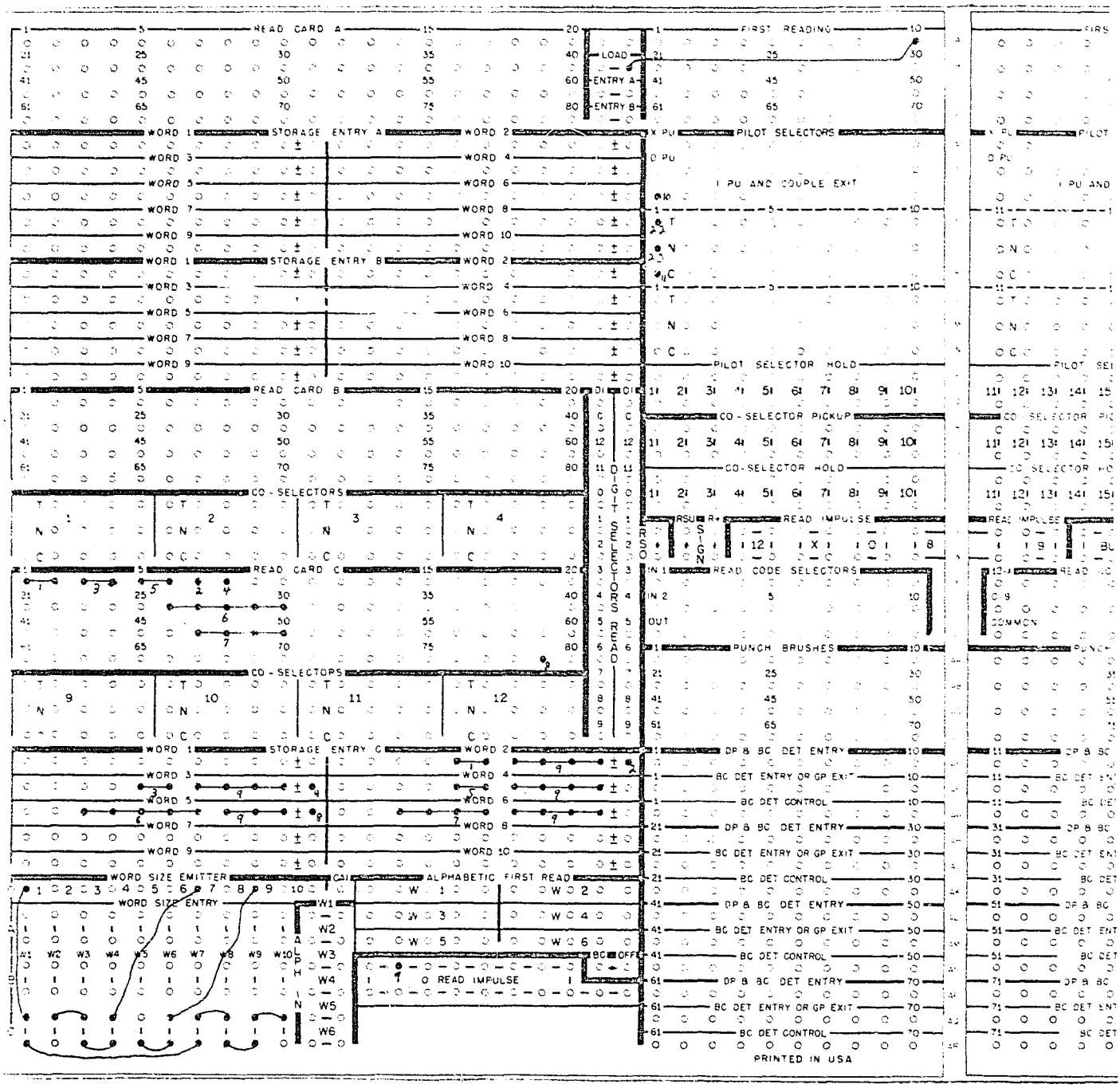


Figure 3. Flow diagram for T.D.F. 80 B program

Figure 4. T.D.F. 80 B wiring diagram for the I.B.M. 650


READ CARD A
LOAD
ENTRY A
ENTRY B
WORD 1
STORAGE ENTRY A
WORD 2
WORD 3
WORD 4
WORD 5
WORD 6
WORD 7
WORD 8
WORD 9
WORD 10
STORAGE ENTRY B
READ CARD B
CO - SELECTORS
READ CARD C
STORAGE ENTRY C
WORD SIZE EMITTER
WORD SIZE ENTRY
ALPHABETIC FIRST READ
READ IMPULSE
BC OFF
FIRST READING
X PU
PILOT SELECTORS
PU AND COUPLE EXIT
PILOT SELECTOR HOLD
CO - SELECTOR PICKUP
CO - SELECTOR HOLD
READ IMPULSE
READ CODE SELECTORS
PUNCH BRUSHES
DP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
PRINTED IN USA

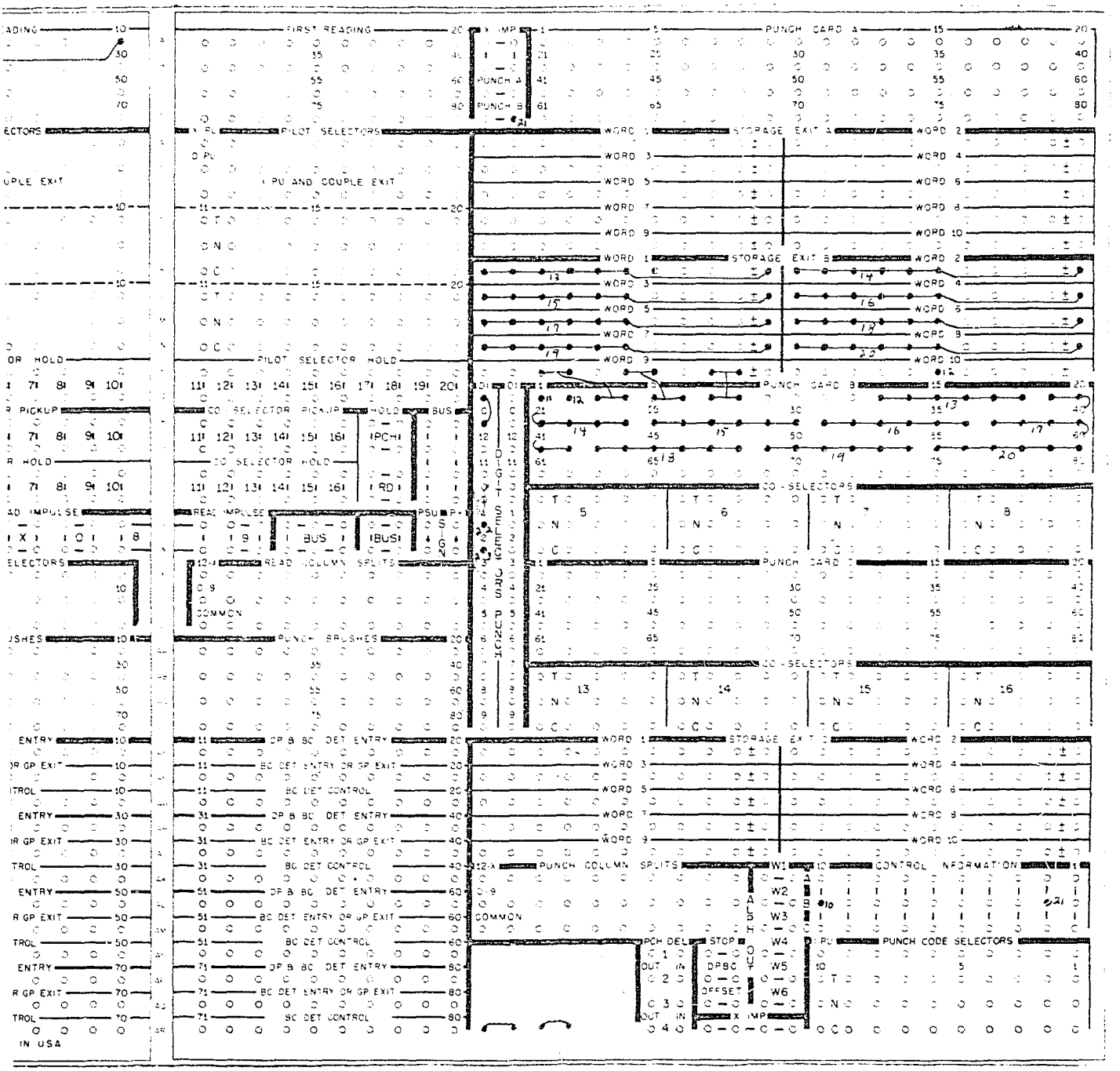

FIRST READING
PUNCH CARD A
PILOT SELECTORS
STORAGE EXIT A
STORAGE EXIT B
PILOT SELECTOR HOLD
CO-SELECTOR PICKUP
CO-SELECTOR HOLD
READ IMPULSE
READ COLUMN SPLITS
PUNCH BRUSHES
DIGIT SELECTORS PUNCH
CO-SELECTORS
PUNCH CARD C
CO-SELECTORS
DP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
PUNCH COLUMN SPLITS
CONTROL INFORMATION
PUNCH CODE SELECTORS
IN USA

TABLE 13. PROGRAM ORDERS FOR T.D.F. 80 B (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0001692020027C	0002099999999I	0003099999999R	0004460007015H
0005241359156B	0006241359161B	0007100010800C	0008100011800C
0010692020032C	0011690021037D	0012111315001I	0013690020067C
0016690036058I	0017101627800C	0018690036183I	0019460022172E
0020099999999I	0022100025800C	0023241127073¤	0024241127078¤
0025692035043H	0026000482043C	0028690036033I	0029460482069G
0030110633003G	0031000083997H	0032200147150¤	0035099999999I
0036099999999R	0037460040009A	0038241342009E	0039241342009F
0040101943800C	0041100044800C	0043692002065E	0044690003065F
0045110899000D	0046110749125E	0047200551021C	0048161656186A
0050100254800C	0051151805180I	0052099691733D	0053099691733M
0054460057030H	0055240109016B	0056240109021B	0057100060800C
0058100061800C	0060692020062C	0061690021042D	0062111365141I
0063690021032D	0066111926078B	0067000014046D	0068690947060¤
0069460122192E	0070099691733D	0071099691733M	0072101376800C
0073241277143¤	0074241277148¤	0075692035058H	0076441929073B
0078690036043I	0079600132098I	0080110683143G	0082004000000¤
0084460890084A	0085099691733D	0086099691733M	0087460090004A
0088241192094E	0089241192024F	0090100043800C	0091100094800C
0093692002035E	0094690003005F	0095110099050D	0096110049130E
0097161810021F	0100600064066I	0101100000019E	0102098768834A
0103098768834J	0104460107071F	0105241209101B	0106241209106B
0107100110800C	0108101868800C	0110692020092C	0111690021007D
0112111165196I	0113690020007C	0116461690149A	0117692036183I
0118000000000¤	0119460172092E	0120098768834A	0121098768834J
0122100075800C	0123240377193¤	0124240377013¤	0125692035088H
0126692036033I	0128690036078I	0129100346800C	0130110283118G
0131240698800C	0132201217122H	0134002000000¤	0135098768834A
0136098768834J	0137460140014A	0138240242024E	0139240242029E
0140100093800C	0141100144800C	0143692002080E	0144690003035F
0145111199005D	0146110949135E	0148151956051C	0150151956086G
0151691410156D	0152097236992¤	0153097236992*	0154460157065H
0155240159026B	0156240159051B	0157100160800C	0158100063800C
0160692020017C	0161690021147D	0162110115006I	0163690020107C
0164160067032H	0166460440067H	0168100628800C	0169461822167D
0170097236992¤	0171097236992*	0172100175800C	0173240327038¤
0174240327043¤	0175692035013H	0176692036108I	0178690036013I
0179240698800C	0180111233013G	0182100892059G	0184460122024H
0185097236992¤	0186097236992*	0187460190019A	0188240292065A
0189240292069F	0190100143800C	0191100194800C	0193692002020E
0194690003080F	0196111049140E	0197461750135D	0200691106185I
0201190354134A	0202095105651F	0203951056510	0204460207060I
0205240409056B	0206240409061B	0207100210800C	0208100161800C
0210692020022C	0211690021052D	0212110165146I	0213161368003B

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0216461874037H		0217240021133B		0218240981123I		0219460222137C	
0220095105651F		0221095105651O		0222100125800C		0223240427053¤	
0224240427058¤		0225692035023H		0226690035003H		0228200581108D	
0229200884133I		0230111283148G		0231200514075G		0232200340186¤	
0234191788030¤		0235095105651F		0236095105651O		0237460240045¤	
0238240442044E		0239240442059F		0240100193800C		0241100944800C	
0243692002175E		0244110401026F		0245110299010D		0246110149145E	
0247201805031C		0248100016800C		0250460422186D		0251016000000¤	
0252092387953B		0253092387953K		0254690021027D		0255241009076B	
0256241009046C		0257100260800C		0258100211800C		0260692020002C	
0261690021062D		0262110315101I		0263690020052C		0264151679191G	
0266461672117D		0267650781143H		0268460740069A		0269460272167C	
0270092387953B		0271092387953K		0272100225800C		0273241027063¤	
0274241027068¤		0275692035028H		0276692036078I		0278451831118B	
0279211195128D		0280111833018G		0282110147155¤		0285092387953B	
0286092387953K		0287460290029A		0288241042059E		0289241042064E	
0290100243800C		0291100294800C		0293692002025E		0294690003105F	
0295110249175D		0296111249190E		0297241805185H		0300201807166D	
0301651807096C		0302089100652D		0303089100652M		0304460257070I	
0305241109091B		0306241109096B		0307100310800C		0308100261800C	
0310692020037C		0311211695151G		0312110715011I		0313200118800¤	
0316161824082I		0317000000005¤		0318600528008D		0319460972172D	
0320089100652D		0321089100652M		0322100275800C		0323240027003¤	
0324240027008¤		0325692035033H		0326690035083H		0328201983163H	
0329211495148D		0330111883183G		0331201801125G		0332690002060E	
0334690020002C		0335089100652D		0336089100652M		0337460840079A	
0338241142069E		0339241142049E		0341100344800C		0343692002030E	
0344690003025F		0345111799015D		0346690002020E		0347450200015A	
0348110401016F		0350101967800C		0351200340030A		0352085264016D	
0353085264016M		0355240209031B		0356240209036B		0357100360800C	
0358100861800C		0360692020042C		0361690020082C		0362110765151I	
0363692035183H		0364151817800C		0366190726036H		0367002000000¤	
0368200478138A		0369460322112C		0370085264016D		0371085264016M	
0372100325800C		0373241227083¤		0374241227048¤		0375692035038H	
0376690036088I		0378160082019G		0379211645158D		0380110333023G	
0382240842100¤		0384651656066F		0385085264016D		0386085264016M	
0387460390034A		0388241242074E		0389241242004F		0390100293800C	
0391101494800C		0393692002010E		0394110401046F		0395111749180D	
0396110849165D		0397241805118D		0400690020092C		0401002000000¤	
0402080901699D		0403080901699M		0404460307000H		0405241309111B	
0406241309116B		0407100410800C		0408100111800C		0410692020047C	
0411690021047D		0412111615021I		0413160167152I		0416111926058B	
0418161926023B		0419461273127E		0420080901699D		0421080901699M	
0422100375800C		0423241327093¤		0424241327098¤		0425692035003H	
0428600781008G		0429211795168D		0430110383158G		0431201001096F	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0432658001128I		0434150987059A		0435080901699D		0436080901699M	
0437460440099G		0438240042004E		0439240042039F		0440100343800C	
0441100444800C		0443692002040E		0444690003010F		0445110499020D	
0446111149170D		0447150401165E		0448100001800C		0450111207061C	
0451201810126D		0452076040596F		0453076040596O		0454460357005H	
0455241409121B		0456241409126B		0457100460800C		0458100461800C	
0460692020142C		0461690021067D		0462111665156I		0463110565166I	
0466461558160I		0467101173800C		0468151375162I		0469460372162E	
0470076040596F		0471076040596O		0472100425800C		0473241427103¤	
0474241427108¤		0475692035048H		0476690036023I		0479211945150D	
0480110783178G		0482151488069G		0485076040596F		0486076040596O	
0487460490044A		0488241442084E		0489241442014F		0490100393800C	
0491100494800C		0493692002045E		0494690003040F		0495110649120E	
0496111349130D		0497201949160D		0500064000000¤		0502070710678A	
0503070710678J		0504460407176D		0505241059131B		0506241059136B	
0507100510800C		0508100761800C		0510692020052C		0511690021072D	
0512110365131I		0513150167063B		0516111926093B		0518461007160H	
0519460422024D		0520070710678A		0521070710678J		0522100475800C	
0523241077123¤		0524241077128¤		0525692035053H		0526650429043D	
0527690035063H		0529201834105¤		0530110433028G		0532151639084G	
0534451938118I		0535070710678A		0536070710678J		0537460540049A	
0538241092089E		0539241092019F		0540100443800C		0541100544800C	
0542200499110E		0543692000205E		0544690003045F		0545460448005¤	
0546111549185E		0548461473001G		0550460922061F		0552064944804H	
0553064944804Q		0554460457020H		0555241159141B		0556241159011B	
0557100560800C		0558650311196E		0560692020057C		0561690021077D	
0562110415026I		0563160367167E		0564160082099H		0566461090127H	
0567241675800C		0568110021007F		0569460472122C		0570064944804H	
0571064944804Q		0572100525800C		0573241177133¤		0574241177138¤	
0575692035008H		0576690036028I		0577690036053I		0578200215182I	
0579000001000¤		0580110483163G		0582460407115A		0585064944804H	
0586064944804Q		0587460590054A		0588240142014E		0589240142044F	
0590100493800C		0591200195199H		0592151095199I		0593692002055E	
0594690003050F		0595110599030D		0596110449115E		0597211953135F	
0598460772191H		0600241675135F		0602058778525B		0603058778525K	
0604460507025H		0605241259146B		0606241259151B		0607100610800C	
0608151863111G		0609101962800C		0610692020007C		0611000033008D	
0612110465161I		0613461140012I		0614690718147H		0616101328800C	
0618461340194B		0619460522097C		0620058778525B		0621058778525K	
0622100575800C		0623240127018¤		0624240127023¤		0625692035063H	
0626690036003I		0627690035018H		0628690003020F		0629150478015¤	
0630110533038G		0631600878193D		0632151807146D		0634151956151C	
0635058778525B		0636058778525K		0637461640104A		0638241292099E	
0639241292029F		0640100543800C		0641100594800C		0642151679089G	
0643692002060E		0644690003055F		0645110549185D		0646111649105D	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0647160500121F		0648461022102C		0650201656170I		0651110399095D	
0652052249856E		0653052249856N		0654460557039D		0655240009001B	
0656240009006B		0657100910800C		0658100661800C		0659100113800C	
0660692020067C		0661690021017D		0662111865041I		0663690020077C	
0664201972162F		0666100878158I		0667461990092H		0668690036073I	
0669460572102D		0670052249856E		0671052249856N		0672100625800C	
0673241377153¤		0674241377158¤		0675692035068H		0676650479043D	
0677690036008I		0678100832800C		0679201742049G		0680110583168G	
0681692036048I		0682000031993B		0685052249856E		0686052249856N	
0687460640064A		0688241392099F		0689241392049F		0690100593800C	
0691100694800C		0692000018006G		0693692002000E		0694690003060F	
0695110699040D		0696110349100D		0697160251160E		0698440951130F	
0700151953061D		0702045399050¤		0703045399050*		0704460607040H	
0705241459166B		0706241459171B		0707100660800C		0708100711800C	
0709100862800C		0710692020072C		0711690021082D		0712111815111I	
0713201267122H		0714690918013A		0716110729098D		0718441582140F	
0719460622192D		0720045399050¤		0721045399050*		0722100675800C	
0723241477163¤		0724241477168¤		0725692035073H		0728110134054H	
0729002000000¤		0730110033043G		0731201141174D		0732101989180F	
0734000015946B		0735045399050¤		0736045399050*		0737460690189A	
0738241492199E		0739241492199F		0740100643800C		0741101094800C	
0742110401056F		0743692002070E		0744690003070F		0745110799045D	
0746111849115D		0747211445150A		0748200354130G		0750000068047¤	
0751101454800C		0752038268343B		0753038268343K		0754460707045H	
0755240059176B		0756240059181B		0757600713076H		0758111863051H	
0759100013800C		0760692020077C		0761692021137D		0762110515036I	
0763200167120¤		0764201972167F		0766241729176F		0767690036038I	
0768691678187I		0769460672177D		0770038268343B		0771038268343K	
0772100725800C		0773240077173¤		0774240077178¤		0775692035108H	
0776650379043D		0777690036063I		0778110134059H		0779241675038D	
0780110083173G		0782460107075A		0785038268343B		0786038268343K	
0787460740074B		0788240092127I		0789240092054F		0790100693800C	
0791100744800C		0792110401026H		0793692002075E		0794690003075F	
0795690002000E		0796200033079G		0797150850095I		0798161922057H	
0802030901699D		0803030901699M		0804461757180H		0805240309041B	
0806240309046B		0807100760800C		0808100811800C		0809101163800C	
0810692020082C		0811690021012D		0812690021137D		0813690818017I	
0814200781183B		0816000016986H		0818441576145F		0819460722152C	
0820030901699D		0821030901699M		0822100775800C		0823240177183¤	
0824240177188¤		0825692035078H		0826690035043H		0827690035093H	
0828110134055¤		0829460532064G		0830110733048G		0831201141199D	
0832690003030F		0834461372177C		0835030901699D		0836030901699M	
0837460790074A		0838240192104E		0839240192064F		0840100743800C	
0841100794800C		0842201684133I		0843692002015E		0844690003015F	
0845110999055D		0846161656022H		0847161800190D		0848200354095H	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0850000001000A		0851101005800C		0852023344536D		0853023344536M	
0854460807173H		0855240259191B		0856240259186B		0857100810800C	
0858100361800C		0859101063800C		0860692020087C		0861692021007D	
0862690021002D		0863150118197C		0864201972172F		0866111926098B	
0867460642089G		0868690229038B		0869460772072H		0870023344536D	
0871023344536M		0872100825800C		0873240277113□		0874240277118□	
0875692036083I		0876690035058H		0877690036068I		0878000000000C	
0879211345138D		0880111983193I		0881690035048H		0882461408191□	
0885023344536D		0886023344536M		0887460990039A		0888240342034E	
0889240342039E		0890100793800C		0891100844800C		0892099691733D	
0893692002085E		0894690003085F		0895111099060D		0896160401135G	
0897691100111F		0898110401066G		0900111899110D		0902015643446E	
0903015643446N		0904460857070H		0905240359071B		0906240359066B	
0907100860800C		0908100911800C		0909101813800C		0910692021082D	
0911690020012C		0912110615046I		0913690020002C		0914460240016H	
0916000515051G		0917191972165G		0918441631160F		0919460822107D	
0920015643446E		0921015643446N		0922100975800C		0923240227028□	
0924240227033□		0925100178800C		0926690035013H		0927690035078H	
0928101682800C		0929240634173I		0930110833053G		0931201141189D	
0932460557158H		0934600340054E		0935015643446E		0936015643446N	
0937460940089A		0938240392090□		0939240392074F		0940100843800C	
0941100894800C		0942200499110F		0943692002090E		0944690002050E	
0945110199065D		0946000017001G		0947200528153A		0948200354185G	
0950151954081C		0951101256036D		0952007845909F		0953007845909O	
0954460907075H		0955240459171D		0956240459121D		0957100960800C	
0958650961196E		0959200083079H		0960692020012C		0961211395131G	
0962110665171I		0963160167062I		0964201972077F		0966913821171I	
0967151679006H		0968241675135F		0969460872112D		0970007845909F	
0971007845909O		0972100276800C		0973101028800C		0974101777800C	
0975692035083H		0976241563021H		0976241563021H		0977690036108I	
0978101132800C		0980110883153G		0982460907168I		0984461507178I	
0985007845909F		0986007845909O		0987000000000□		0988160946085A	
0989151952800C		0990101043800C		0991101828800C		0992240698800□	
0993692002095E		0995111299070D		0996111399075D		0997110401011F	
0998461251105E		1000151955071D		1002000000000□		1003000000000□	
1004461007086F		1005000031948□		1005000031948□		1006161963046G	
1007101260800C		1008101011800C		1010151863171G		1011690020032C	
1012110215051I		1013110816800C		1014461067041H		1016101128800C	
1017000000000□		1018241150170F		1019460922122D		1020000000000□	
1021000000000□		1022100875800C		1023100326800C		1024100577800C	
1025101378800C		1026690035088H		1028690036048I		1029692003190F	
1030110933058G		1031201141194D		1032240987118D		1034692035023H	
1035000000000□		1036000000000□		1037461790094A		1038161441114F	
1039100542004H		1040100943800C		1041101044800C		1043692003015F	
1044690002085E		1045111699090D		1046111450155E		1047211295140A	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1048200354055H		1050601413086H		1051691656076F		10520078459090	
1053007845909F		1054460657085H		1055160367123A		1056240509099D	
1057101816800C		1058101061800C		1060692021032D		1061690020062C	
10621102651761		1063690020022C		1064201972052F		1066101079800C	
10671519260238		1068201999110F		1069461072132D		10700078459090	
1071007845909F		1072101125800C		1073240477028B		1074100977800C	
1075690002095E		1076690035023H		1078692002190F		1079690002190F	
1080110983188G		1084151138174C		10850078459090		1086007845909F	
1087461040099A		1088241592080□		1089241592080□		1090101993800C	
1091101144800C		1093692003085F		1094690003000F		1095004000000□	
1096110551187H		1097211745170A		1098160401170E		1099692035053H	
1100200064176G		1101150916052I		1102015643446N		1103015643446E	
1104460957080H		1105161908151D		1106000001000□		1107000003000□	
1108651161196E		1110692021062D		1111690020017C		1112110815056I	
1113200014122H		1114190317152H		1116241675135F		1117200781188H	
1119461222102E		1120015643446N		1121015643446E		1122101326800C	
1123100576800C		1124100128800C		1125692035018H		1126690035028H	
1128690003190F		1130111733108G		1131201141184D		1132200099110E	
1134151138004G		1135015643446N		1136015643446E		1137461990169A	
1138000033088C		1140101193800C		1143692003090F		1144690002070E	
1145161949155D		1146110750800C		1147211895180A		1148200354110H	
1150151956018B		1151100411800C		1152023344536M		1153023344536D	
1154461057090H		1155461208085I		1156601460036F		1158101111800C	
1160692021092D		1161211845161G		1162110865181I		1163690020042C	
1164201972067F		1166000482043C		1167099691733M		1169460072152D	
1170023344536M		1171023344536D		1172101476800C		1173000034003B	
1174101877800C		1175692035093H		1176110729018D		1178200987024G	
1179240842196D		1180111783128G		1181240842070□		1182651538084F	
1184650340114E		1185023344536M		1186023344536D		1187461340089H	
1189691642029G		1190101243800C		1193692003020F		1194690002090E	
1200601954161D		1201690021057D		1202030901699M		1203030901699D	
1204221657136□		1205461308090I		1206150611101C		1207002000000□	
1208101211800C		1210692021017D		1211692021022D		1212110915061I	
1213690020047C		1214111081188I		1216461660126F		1218200183190□	
1219461473077H		1220030901699M		1221030901699D		1222101175800C	
1223100626800C		1224110134064H		1225692036043I		1226241788800□	
1228100031193B		1229240987135□		1230111033068G		1231150334079F	
1235030901699M		1236030901699D		1237461090079B		1238151941800C	
1239240547188B		1240101493800C		1241101294800C		1243692003070F	
1244690002005E		1250191810076C		1251150367123A		1252038268343K	
1253038268343B		1254690021087D		1255461358080I		1256201717122I	
1257601113186G		1258100913800C		1260692021087D		1261692021002D	
1262110965186I		1263690020142C		1264651167162H		1266161825002I	
1269461272097D		1270038268343K		1271038268343B		1272100176800C	
1273101526800C		1274101927800C		1275100827800C		1276692036008I	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1278100332800C		1279111599085D		1280111083193G		1281161742044G	
1285038268343K		1286038268343B		1287461290184A		1288461992150E	
1289350001064G		1290101143800C		1291101344800C		1293692003000F	
1294690002035E		1300240021168H		1302045399050*		1303045399050¤	
1304461658075I		1305461408041F		1306651952142I		1307651610196E	
1308101361800C		1310100163800C		1311211545141G		1312111015071I	
1313064000000¤		1314691017161H		1316200149161F		1318200065042H	
1319461022062H		1320045399050*		1321045399050¤		1322101225800C	
1323101126800C		1324101728800C		1325692036013I		1326692036063I	
1328690036083I		1329000000995A		1330111133073G		1331691068177H	
1332690942175F		1335045399050*		1336045399050¤		1337461190109A	
1338110842069H		1340101593800C		1343692003005F		1344690002080E	
1350241805118D		1352052249856N		1353052249856E		1354161207140D	
1355461458150I		1356300001131D		1357200064026G		1358101411800C	
1360601563091G		1361692021037D		1362111065016I		1363690020057C	
1364240150195E		1366150850121H		1368000016076F		1369461172142D	
1370052249856N		1371052249856E		1372101976800C		1373100376800C	
1374240477088¤		1375000033003C		1376692036068I		1378690036093I	
1379151166043A		1380111183198G		1381601234125¤		1382201684133I	
1385052249856N		1386052249856E		1387461590179A		1388213411139D	
1389460592199I		1390101343800C		1391101444800C		1393692003035F	
1394600547020A		1400100117800C		1402058778525K		1403058778525B	
1404151707166A		1405461508155I		1406651953155F		1407101060800C	
1408101461800C		1410000002000¤		1411692021042D		1412111115076I	
1413200417122H		1414161926148A		1418601952151¤		1419461322172C	
1420058778525K		1421058778525B		1422101325800C		1423241527028D	
1424100627800C		1425692036088I		1426692036073I		1428200481133I	
1429150026033A		1430110133078G		1431160134148I		1432691952101H	
1435058778525K		1436058778525B		1437461390199A		1438151742109H	
1440101393800C		1441000019001I		1443692003080F		1444690002175E	
1452064944804Q		1453064944804H		1454690021092D		1455461558051F	
1456651954110A		1457101110800C		1458101511800C		1461692021047D	
1462111215081I		1463690020072C		1464460967006H		1466201767122I	
1468200514122I		1469461372117F		1470064944804Q		1471064944804H	
1472101425800C		1473101426800C		1474241527028D		1475150478115¤	
1476692036018I		1478240698800C		1479000016001F		1480110183123G	
1481200528042H		1482000500050¤		1485064944804Q		1486064944804H	
1487461440124A		1488032000000¤		1489461792089F		1490101443800C	
1491101544800C		1493692003105F		1494690002015E		1500690814077I	
1502070710678J		1503070710678A		1504661107086C		1505100018800C	
1506461759176¤		1507101160800C		1508101561800C		1509101263800C	
1510190317138I		1511692021147D		1512111265116I		1513460264191G	
1514111968800C		1516151810056D		1518200917122I		1519461422182C	
1520070710678J		1521070710678A		1522101525800C		1523100877800C	
1524101577800C		1525692036023I		1526692036093I		1528691581130¤	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1529160478063D		1530111333083G		1531691955097F		1532200133136F	
1535070710678J		1536070710678A		1537461540159A		1538692002095E	
1540101543800C		1541101594800C		1542000018041H		1543692003040F	
1544690002030E		1550461911101F		1552076040596O		1553076040596F	
1554151207101D		1555460108177I		1556151482023A		1557101210800C	
1558101611800C		1559100263800C		1561692021052D		1562110015086I	
1564240118178A		1566161329163B		1569461472187C		1570076040596O	
1571076040596F		1572101575800C		1573200727173A		1575692036028I	
1576101466036D		1577690035068H		1578100881800C		1580111383138G	
1581201815056I		1582101468036D		1585076040596O		1586076040596F	
1587461140167G		1588101201800C		1589168002170¤		1590101293800C	
1591101644800C		1593692003095F		1594690002010E		1600101029800C	
1602080901699M		1603080901699D		1604601953111D		1605461758031F	
1606651955137I		1607101261800C		1608101811800C		1609101363800C	
1610211245121G		1611692021057D		1612110065121I		1614190317065¤	
1616161479153B		1618220027043B		1619461522192C		1620080901699M	
1621080901699D		1622100126800C		1623100226800C		1624200099171C	
1625100028800C		1626650279043D		1627690035073H		1628201952115F	
1629110734800C		1630111433033G		1631101518036D		1632200199166F	
1635080901699M		1636080901699D		1637461240139A		1638161542165¤	
1639008000000¤		1640101093800C		1641101694800C		1642000003000¤	
1643692003030F		1644690002040E		1650201081113D		1652085264016M	
1653085264016D		1654461407100H		1655461010141D		1658101914800C	
1659100663800C		1660151313126F		1661691814021G		1662111415091I	
1663690035183H		1664150167147E		1666150850131F		1669461572132C	
1670085264016M		1671085264016D		1672101775800C		1673100476800C	
1674101727800C		1675200781183B		1676650879043D		1677111207091D	
1678201734133I		1679960000000¤		1680111483133G		1681200015185A	
1682690003095F		1685085264016M		1686085264016D		1687460350196F	
1688461842045A		1689101254800C		1690101643800C		1691111207061H	
1692000001000¤		1693692003010F		1694690002045E		1700198001009G	
1702089100652M		1703089100652D		1704461457105H		1705460608190I	
1706691953092I		1707690035003H		1708101761800C		1709608002023D	
1710002000000¤		1711692021072D		1712111465126I		1713150850176C	
1714110581128H		1716000019006I		1717200528042H		17194616221270	
1720089100652M		1721089100652D		1722101875800C		1723100826800C	
1724100927800C		1725100078800C		1726650329043D		1727690035008H	
1728690036018I		1729002000000¤		1730111533093G		1731691784138H	
1732200265177B		1735089100652M		1736089100652D		1737461690034H	
1738100561800C		1739691954136D		1740101693800C		1741101794800C	
1743201450016D		1744651047005A		1750151207140D		1752092387953K	
1753092387953B		1754461507006F		1755240509099D		1756241933097H	
1757100710800C		1758151961031F		1759101711800C		1760101463800C	
1761692021077D		1762111515096I		1763200049156F		1764111926088B	
1766200021133A		1767660478014H		1768161729178B		1769461672188A	

TABLE 13. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1770092387953K		1771092387953B		1772150682162D		1773100876800C	
1774100777800C		1775692036038I		1777690035108H		1778241933063A	
1779100812800C		1780111583088G		1781240987039G		1782451931150□	
1784100000072G		1785092387953K		1786092387953B		1787461740154A	
1789100400800C		1790100893800C		1791100795800C		1792150401135G	
1793692003045F		1794690002055E		1800004000000□		1802095105651O	
1803095105651F		1804461557115H		1805000000000□		1806161815027H	
1808100511800C		1809201913191F		1811690020087C		1812111565031I	
1813690020037C		1814200315056I		1816692021012D		1817000085008C	
1818150726143A		1819461722162C		1820951056510		1821095105651F	
1822101276800C		1823100926800C		1824008000000□		1825032000000□	
1826690002025E		1827100681800C		1828690003090F		1829150850173B	
1971099691733D		1973451876117H		1974100527800C		1976692036058I	
1985099691733M		1986099691733D		1987461940174A		1988191141197E	
1989000000000A		1990100993800C		1991101244800C		1992100363800C	
1997211595160A		1998690101120D		1999200726067I		1996111449150F	
1830111633103G		1831651892105A		1832651807041C		1835095105651O	
1836095105651F		1837461490129A		1838240492104F		1839240492109F	
1840101793800C		1841101194800C		1842151095045A		1843692003050F	
1844651147005A		1850440951130F		1851150850131H		1852097236992*	
1853097236992□		1854461607125H		1855461708165I		1857651311196E	
1858240118103B		1859240118122I		1860650064181H		1861690814056G	
1862111765136I		1863002000000□		1864100767800C		1867691428118A	
1868692020107C		1869461827157H		1870097236992*		1871097236992□	
1872221975192H		1873101026800C		1874150134140D		1875692036003I	
1876150579053D		1877690035038H		1878460508131□		1879240842095□	
1880111683063G		1881110134025□		1882651656176H		1885097236992*	
1886097236992□		1887461840164A		1888650528128A		1889461400190A	
1890101843800C		1891100644800C		1892099999999R		1893692003055F	
1894651997005A		1900161716168A		1901101663800C		1902098768834J	
1903098768834A		1904461907056C		1905460358065I		1906240559130A	
1907151710167E		1908000015001E		1909161863111G		1910101213800C	
1911101078800C		1912111715106I		1914692021067D		1916691919187B	
1917690351096H		1918100668800C		1919100000191C		1920098768834J	
1921098768834A		1922000018991I		1923101076800C		1924100677800C	
1925110729083D		1926002000000□		1927690035033H		1928600981198H	
1929101933123H		1930110233113G		1931651034103I		1932160692800C	
1933201999110F		1934191656151F		1935098768834J		1936098768834A	
1937461890024A		1938151692034G		1939461600106F		1940101893800C	
1941000033008C		1942101075800C		1943692002005E		1944651097005A	
1952099691733M		1953099691733D		1961016000000□		1962690021022D	
1963000015001E		1964691850099B		1965150118157C		1966101826800C	
1967692003025F		1968000066011G		1969461122197D		1970099691733M	
1993692003060F		1994650747005A		1995111499080D		1996111449150F	

TABLE 14. PROGRAM ORDERS FOR T.D.F. 80 B PUNCH (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0009651460002G		0027350003004B		0042151234010I		0109350003012G	
0127151788014B		0142201985020I		0209650059007G		0059691195800C	
0077100092800B		0092241977019B		0192690227024B		0227240000025I	
0242220277029B		0292691017027G		0259110309032G		0309241984019C	
0327440342035I		0342100377039B		0377241985019C		0392150409800B	
0409000050000¤		0359101989042G		0427160442055I		0442001544000¤	
0559691009102G		1009800000008¤		1027221986104B		1042150442105I	
1059711977107G		1077150409109B		1092100092110I		1109691127114B	
1127440342115I		1142240327800B		1159101989147G		1477161192120I	
1192001944000¤		1209691227124B		1227900000008¤		1242221986125I	
1259151192127G		1277711977129B		1292161309135I		1309691948800C	
1359451377139B		1377151342140I		1342691199800C		1409100092142G	
1427691442145I		1442440342035I		1459240327800B		1392701951141H	

VIII. APPENDIX B: T.D.F. 40-80 PROGRAM FOR I.B.M. 650

A. Fourier Series Evaluation on a Grid Spacing of 1/40 or 1/80 of the Unit Cell

1. Function to be evaluated

The three dimensional Fourier series for the electron density is evaluated in the form

$$\rho(xyz) = \sum_{\ell=0}^{+\infty} \sum_{k=0}^{+\infty} \sum_{h=0}^{+\infty} \Big[A_1(hk\ell) \cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z + A_2(hk\ell) \sin 2\pi hx \sin 2\pi ky \cos 2\pi \ell z + A_3(hk\ell) \sin 2\pi hx \cos 2\pi ky \sin 2\pi \ell z + A_4(hk\ell) \cos 2\pi hx \sin 2\pi ky \sin 2\pi \ell z + B_1(hk\ell) \sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z + B_2(hk\ell) \cos 2\pi hx \cos 2\pi ky \sin 2\pi \ell z + B_3(hk\ell) \cos 2\pi hx \sin 2\pi ky \cos 2\pi \ell z + B_4(hk\ell) \sin 2\pi hx \cos 2\pi ky \cos 2\pi \ell z \Big]$$

where

$$\begin{aligned}
A_1 &= A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_2 &= -A'(hk\ell) - A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_3 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) - A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_4 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) - A'(\bar{h}k\ell) \\
B_1 &= -B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_2 &= B'(hk\ell) + B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_3 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) - B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_4 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) - B'(\bar{h}k\ell)
\end{aligned}$$

and where A' and B' refer to the real and imaginary parts of the structure factor, multiplied by the appropriate multiplicity factor. For general structure factors, the factor is $\frac{2}{V}$. For structure factors having n zero indices, the factor is $\frac{2^{1-n}}{V}$. The special reflections are best handled by leaving out the required proportion of the coefficients.

The evaluation is carried out by successive one dimensional summations. The function is evaluated at intervals of either 1/80 or 1/40 of the unit cell. Two dimensional projections can be calculated by stopping after two summations.

2. Method of evaluation

The function is evaluated only over x = 0,1/4, y = 0,1/4 and z = 0,1/4. The remainder of the cell is obtained by tabular expansion.

Trigonometric decks containing cos 2πhx and sin 2πhx for h = 1,2,...,39 and x = 1/80, 2/80,...,19/80 (or, for the 1/40 case, x = 1/40,2/40,...,10/40) are loaded onto the drum. The program forms the products and sums required for a one dimensional summation. The results may be punched in a format suitable for another summation or they may be punched in a format suitable for tabulation. If another summation is not required the results are punched out with 11 points per card. In the 1/80 case, two ranges are required. The first range contains the points 0/80,1/80,...,10/80. The second

range contains the points 11/80,...,20/80. It should be noted that the h,k and ℓ designations of the card fields are arbitrary but that the resultant x,y,z designations are defined in terms of the h,k,ℓ designations. It may be more efficient to change the h,k,ℓ designations in a particular problem.

Since the calculation is to be made with fixed decimal point, it may be necessary to use a scaling factor for the initial data. The coefficients are read onto the drum as xxxx.xxoooo. They are multiplied by 6 figure sin and cos (as .xxxxxxoooo). The upper accumulator is then stored. The last 4 digits of the product are carried during the summation but are dropped just before the punching operation. This leaves a maximum of 6 digits to be fed back for the next sum. The decimal point in the cards for tabulation is xxxx.xx. The extreme left hand digit should be 0. It is carried primarily as an overflow indication. The tabulator prints only xxx.xx.

3. Method of expansion

The expansion to the remainder of the unit cell is carried out on a Type 402 tabulator. The tabulation is based on the fact that $\left.\begin{matrix}\cos\\ \sin\end{matrix}\right\} 2\pi(hx + \frac{hn}{4})$ may be evaluated in terms of the values obtained in the first 1/4 x 1/4 x 1/4 block of the unit cell. This is shown in Table 15.

Table 15. Transformation of cos and sin by n/4

n	h even	h odd	h even	h odd
0	cos $2\pi hx$	cos $2\pi hx$	sin $2\pi hx$	sin $2\pi hx$
1	cos $2\pi hx'$[a]	-cos $2\pi hx'$[a]	-sin $2\pi hx'$[a]	sin $2\pi hx'$[a]
2	cos $2\pi hx$	-cos $2\pi hx$	sin $2\pi hx$	-sin $2\pi hx$
3	cos $2\pi hx'$[a]	cos $2\pi hx'$[a]	-sin $2\pi hx'$[a]	-sin $2\pi hx'$[a]

[a]Note that $x' = 1/4 - x$.

This expansion requires that the series be broken up into subseries during the I.B.M. 650 calculation. All terms of a given subseries must transform in the same way under a coordinate translation of n/4 in each direction (n = integer). In general the subseries must contain only terms having the same form of the trigonometric part and having the same evenness or oddness of each index. There are 64 possible subseries which can occur. If a completely general expansion is not required, it may be possible to combine certain subseries that transform similarly under the translations that are to be used. For a two dimensional summation, the maximum number of possible subseries is 8.

In order to generate these subseries, the detail cards must be sorted into subseries groups before a summation is

carried out. They must also be sorted, within subseries groups, on the indices not being summed over.

Consequently, by changing the signs of the various subseries in the manner shown above, the summation on the 402 can generate the remaining 3/4 cycle in each direction from the results of the first 1/4 cycle. Note that, when n = 2m+ 1, the transformation x' = 1/4 - x requires that the x' coordinate represent the lattice point. This means that the tabulated coordinates (from 0 to 1/4) must be translated and read in reverse.

The wiring changes required for the various blocks of the unit cell can be made by hand. However, in a full capacity Type 402, the various translations may be obtained by three, externally mounted, 4p4t rotary switches. The desired translations are then dialed on the switches. In conjunction with 4 pilot selectors, each switch determines the proper sign of one of the 3 factors that form the subseries. These 3 signs are then multiplied by the coselectors and used to control the counters for algebraic addition or subtraction. If it is desired, it can be so arranged that a heading card prints a code that designates the required switch setting and also tests the switch settings by printing, in the same code, the actual switch settings. The use of the heading card was found to be inconvenient in practice and no errors have resulted from not using this procedure.

4. Flow diagram, wiring information, and speed

The flow diagram for the T.D.F. 40-80 program is given in Figure 5. Zero indices are treated in a special manner in order to speed up the card reading rate.

The wiring diagrams for the I.B.M. 650 and 402 are given in Figures 6 and 7 respectively. The I.B.M. 650 wiring board uses storage entry C for input of detail cards, storage exit A for output of single coefficient cards, and storage exit C for output of multiple coefficient cards.

The detail cards will be read at a rate of approximately 100 cards per minute and the output cards will be punched at the maximum rate of 100 cards per minute. The internal calculations themselves require a negligible amount of time.

B. Operating Instructions

1. Card formats

The formats of the input detail cards at the various stages of the calculation are given in Table 16.

The formats of the multiple coefficient output cards at the various stages of the calculation are given in Table 17.

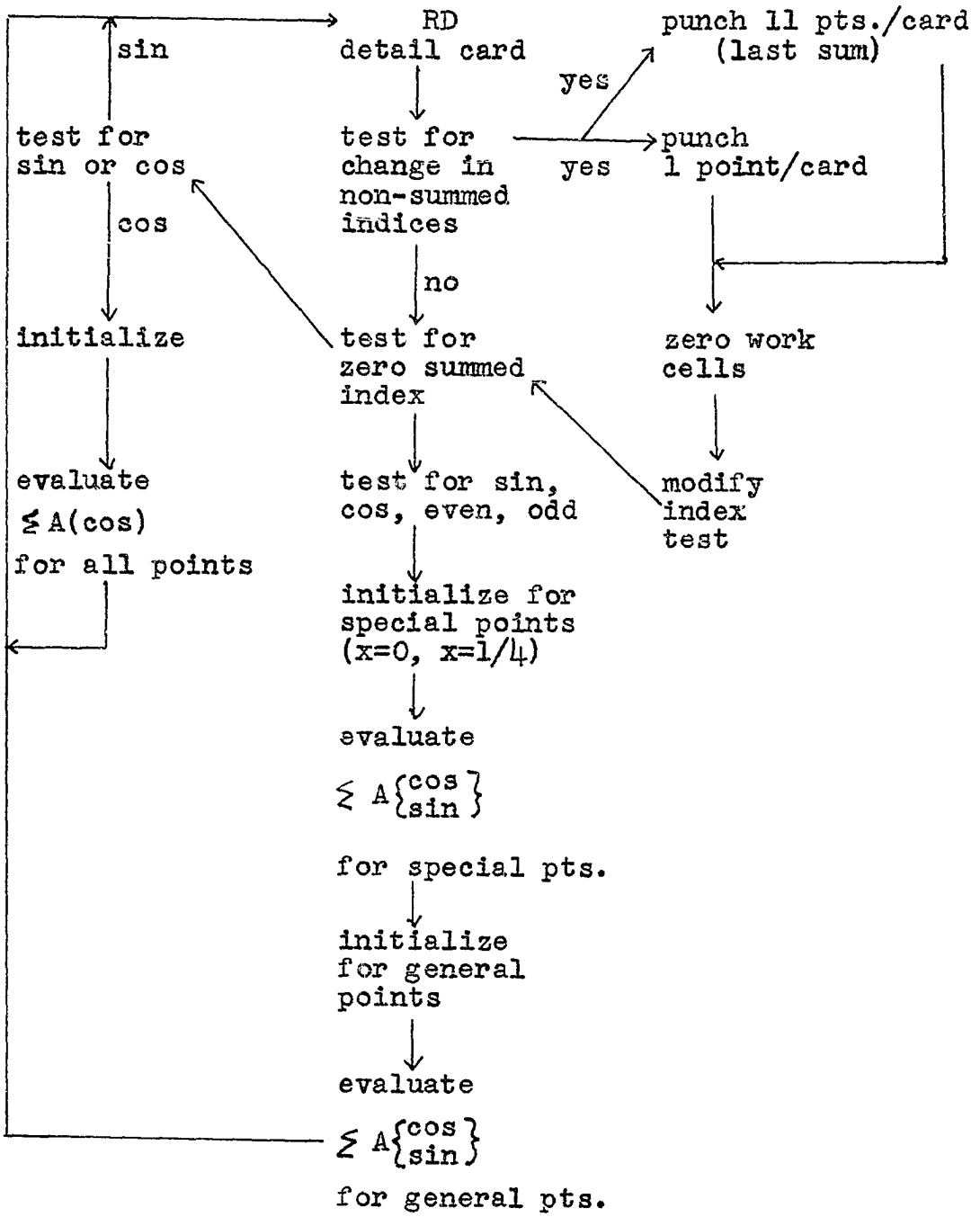
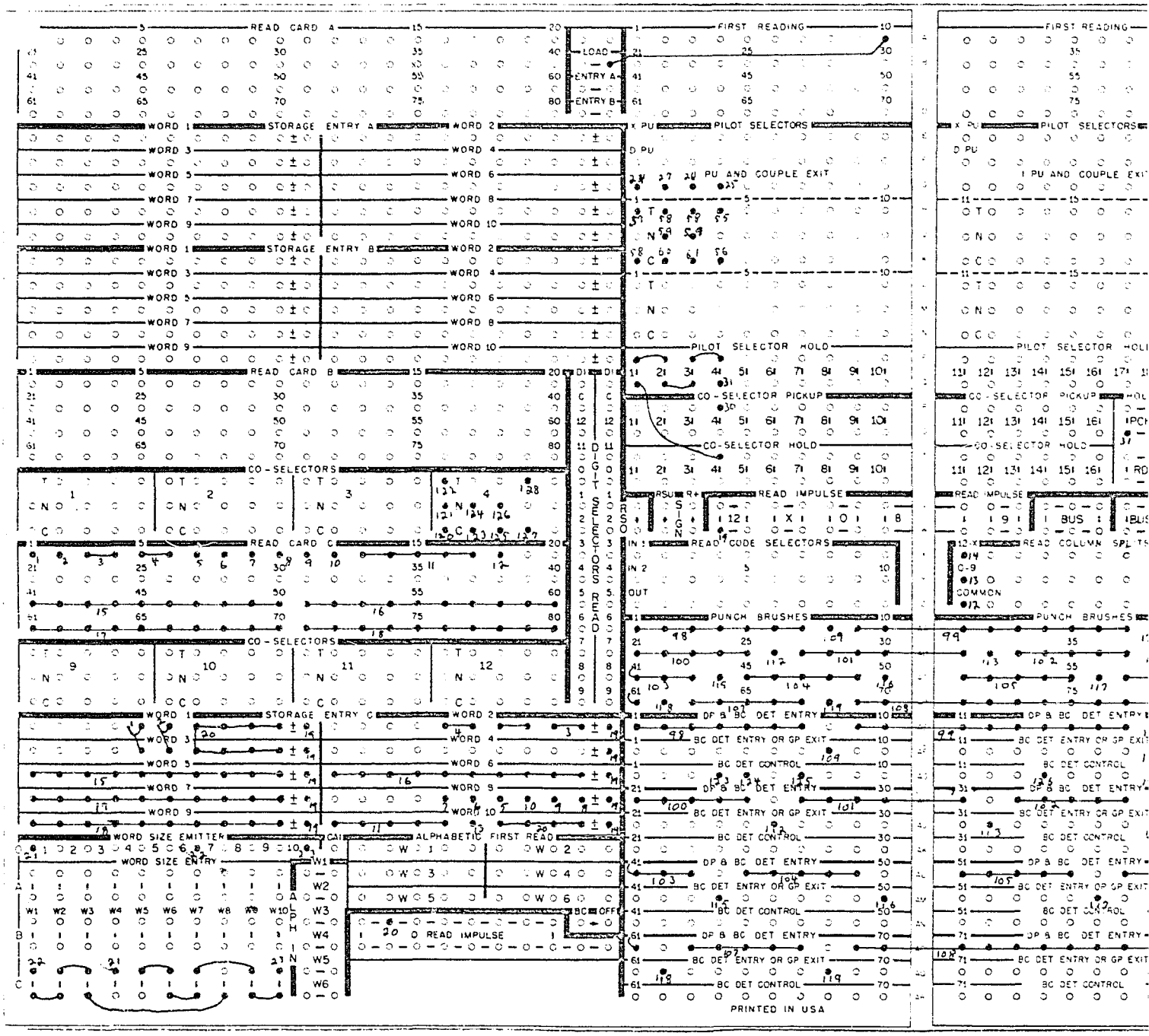


Figure 5. Flow diagram for T.D.F. 40-80

Figure 6. I.B.M. 650 plug board diagram for the T.D.F. 40-80 program


READ CARD A
LOAD
ENTRY A
ENTRY B
STORAGE ENTRY A
STORAGE ENTRY B
READ CARD B
CO-SELECTORS
READ CARD C
STORAGE ENTRY C
WORD SIZE EMITTER
WORD SIZE ENTRY
ALPHABETIC FIRST READ
READ IMPULSE
FIRST READING
PILOT SELECTORS
PU AND COUPLE EXIT
PILOT SELECTOR HOLD
CO-SELECTOR PICKUP
CO-SELECTOR HOLD
READ IMPULSE
READ CODE SELECTORS
PUNCH BRUSHES
DP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
DIGIT SELECTORS READ
PRINTED IN USA

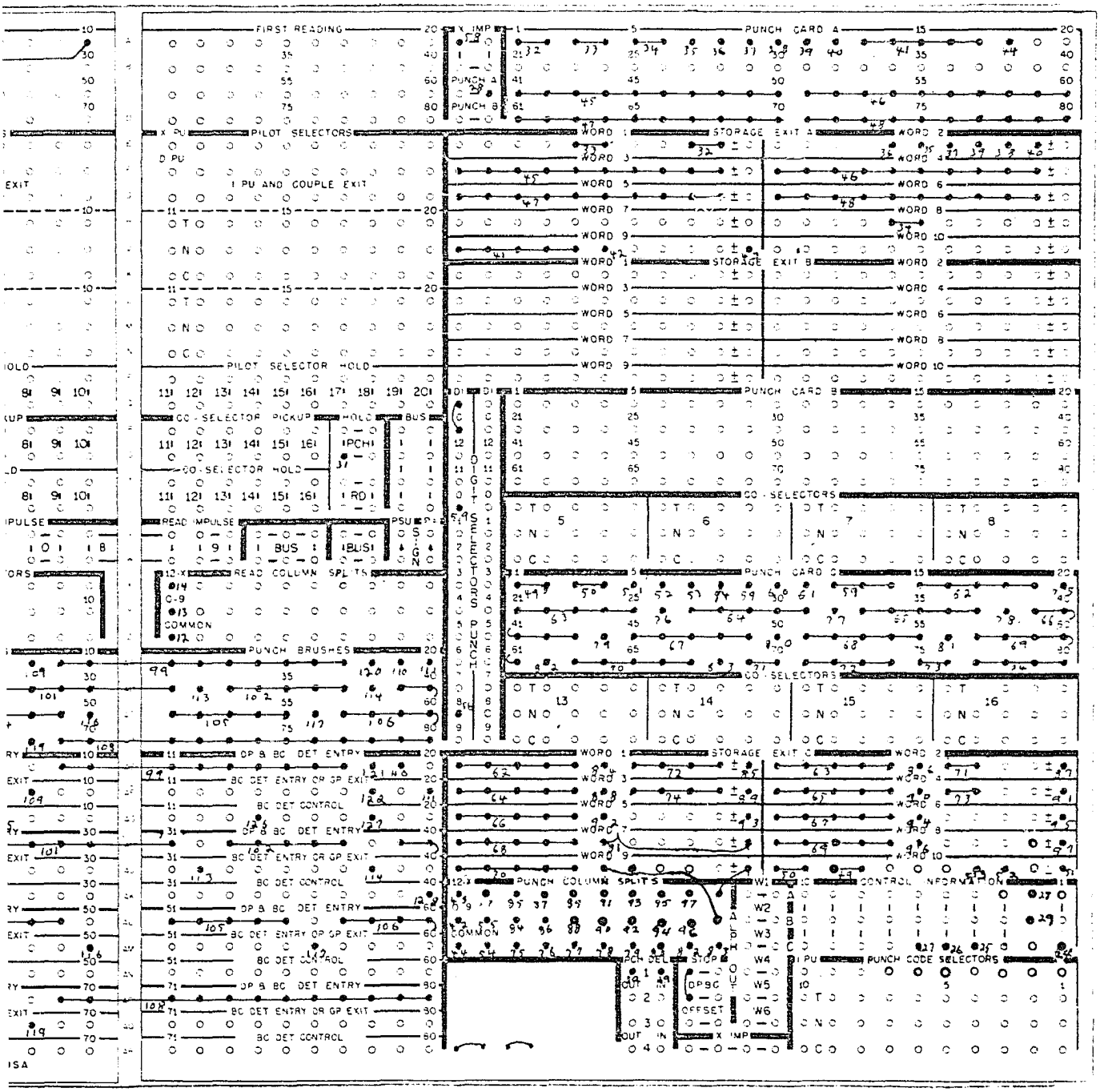
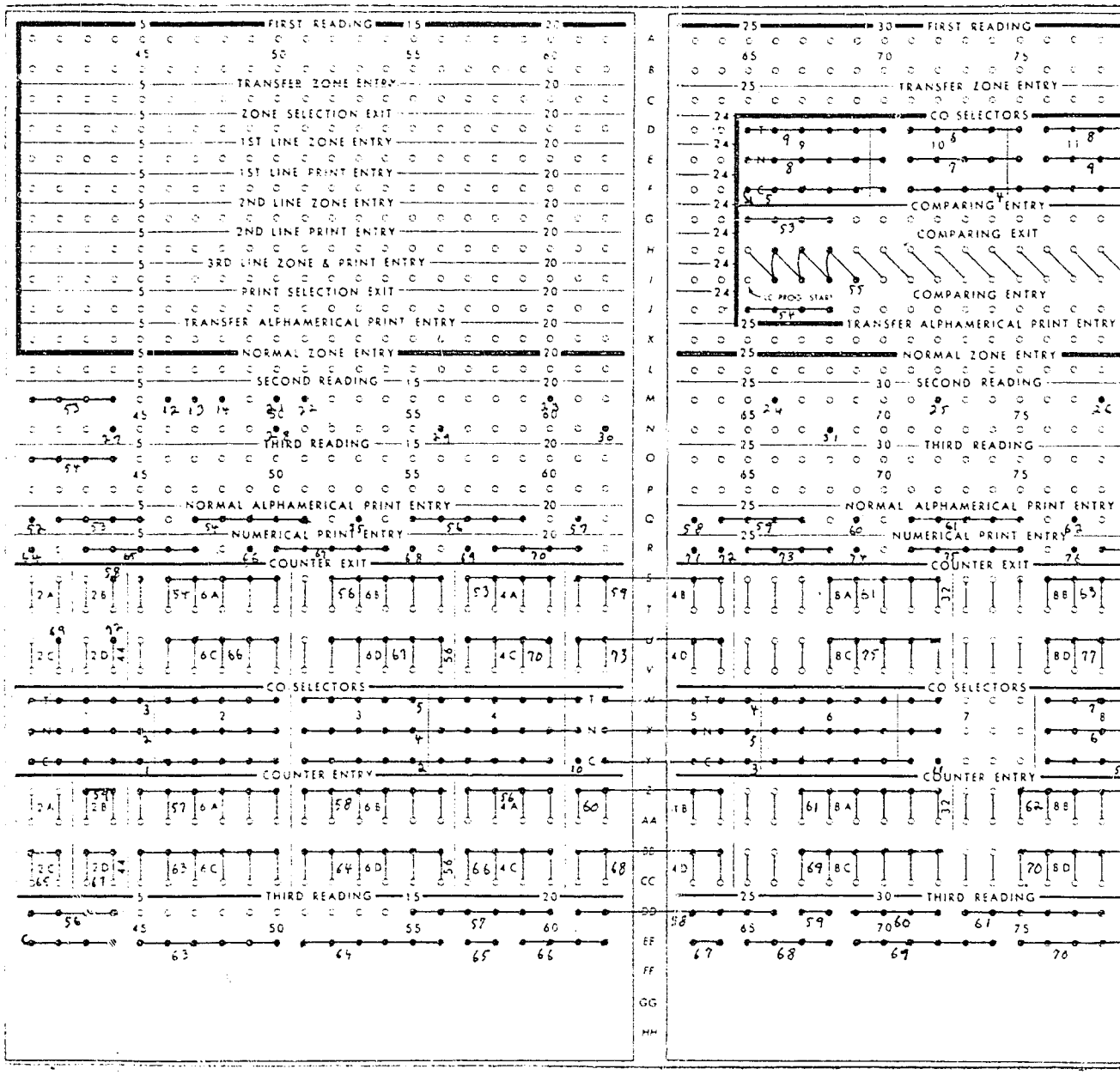

FIRST READING
X IMP
PUNCH CARD A
PUNCH A
PUNCH B
X PU
PILOT SELECTORS
D PU
I PU AND COUPLE EXIT
WORD 1
STORAGE EXIT A
WORD 2
WORD 3
WORD 4
WORD 5
WORD 6
WORD 7
WORD 8
WORD 9
WORD 10
STORAGE EXIT B
PILOT SELECTOR HOLD
PUNCH CARD B
CO-SELECTOR PICKUP
HOLD
BUS
CO-SELECTOR HOLD
IPCHI
IRDI
IBUSI
CO-SELECTORS
READ IMPULSE
PSU
BUS
READ COLUMN SPLITS
COMMON
PUNCH CARD C
PUNCH BRUSHES
OP B BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
PUNCH COLUMN SPLITS
CONTROL INFORMATION
PUNCH CODE SELECTORS
DIGIT SELECTORS PUNCH
OUT IN
DP BC
OFFSET
X IMP

Figure 7. I.B.M. 402 plug board diagram for the T.D.F. 40-80 program


FIRST READING
TRANSFER ZONE ENTRY
ZONE SELECTION EXIT
1ST LINE ZONE ENTRY
1ST LINE PRINT ENTRY
2ND LINE ZONE ENTRY
2ND LINE PRINT ENTRY
3RD LINE ZONE & PRINT ENTRY
PRINT SELECTION EXIT
TRANSFER ALPHAMERICAL PRINT ENTRY
NORMAL ZONE ENTRY
SECOND READING
THIRD READING
NORMAL ALPHAMERICAL PRINT ENTRY
NUMERICAL PRINT ENTRY
COUNTER EXIT
CO SELECTORS
COUNTER ENTRY
THIRD READING
CO SELECTORS
COMPARING ENTRY
COMPARING EXIT
LC PROG. START
COMPARING ENTRY
TRANSFER ALPHAMERICAL PRINT ENTRY
NORMAL ZONE ENTRY
SECOND READING
THIRD READING
NORMAL ALPHAMERICAL PRINT ENTRY
NUMERICAL PRINT ENTRY
COUNTER EXIT
CO SELECTORS
COUNTER ENTRY
THIRD READING

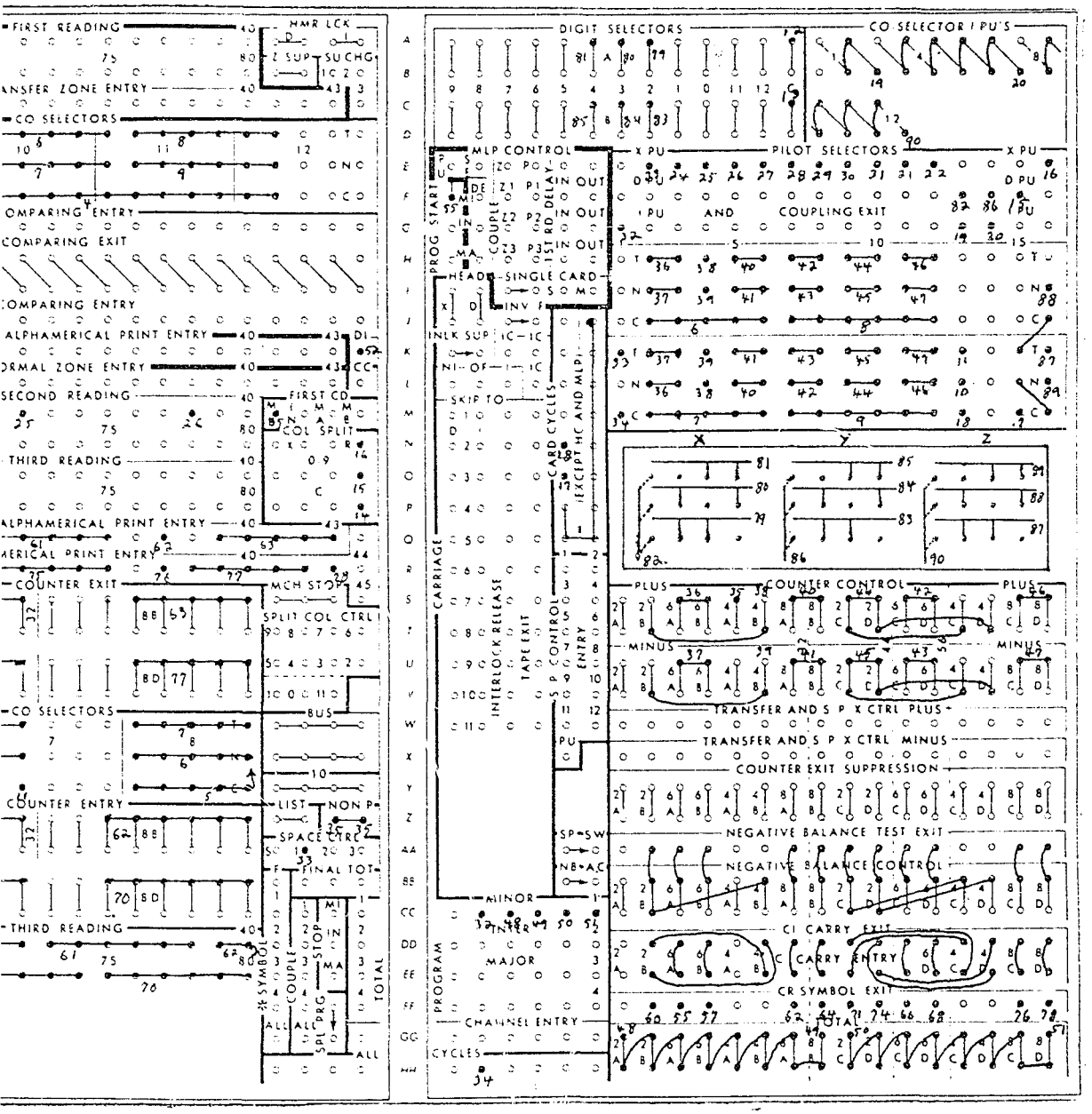

FIRST READING
NMR LCK
Z SUP
SUCHG
TRANSFER ZONE ENTRY
CO SELECTORS
COMPARING ENTRY
COMPARING EXIT
COMPARING ENTRY
ALPHAMERICAL PRINT ENTRY
NORMAL ZONE ENTRY
SECOND READING
FIRST CD
COL SPLIT
THIRD READING
ALPHAMERICAL PRINT ENTRY
NUMERICAL PRINT ENTRY
COUNTER EXIT
MCH STOP
SPLIT COL CTRL
CO SELECTORS
BUS
COUNTER ENTRY
LIST
NON P
SPACE CTRL
FINAL TOT
THIRD READING
SYMBOL
COUPLE
STOP
MA
PRO
ALL
TOTAL
DIGIT SELECTORS
CO SELECTOR I PU'S
MLP CONTROL
X PU
PILOT SELECTORS
I PU AND COUPLING EXIT
PROG START
COUPLE
Z1 P1
Z2 P2
Z3 P3
1ST RD DELAY
IN OUT
HEAD
SINGLE CARD
INV F
INLK SUP
SKIP TO
CARD CYCLES
EXCEPT HC AND MLP
CARRIAGE
INTERLOCK RELEASE
TAPE EXIT
S P CONTROL
ENTRY
PU
SP-SW
NB-AC
MINOR
INTERM
MAJOR
PROGRAM
CHANNEL ENTRY
CYCLES
X
Y
Z
PLUS
COUNTER CONTROL
MINUS
TRANSFER AND S P X CTRL PLUS
TRANSFER AND S P X CTRL MINUS
COUNTER EXIT SUPPRESSION
NEGATIVE BALANCE TEST EXIT
NEGATIVE BALANCE CONTROL
CI CARRY EXIT
CARRY ENTRY
CR SYMBOL EXIT
TOTA

Table 16. Input detail cards and single coefficient output cards

Card col.	Contents 1st sum	2nd sum	3rd sum	Comments
1-2	h	k	ℓ	Summation occurs over the index in col. 1-2
3-4	k	ℓ	x	
5-6	ℓ	x	y	
7	α_h	α_k	α	$\alpha_i = 8$ if i is even
8	α_k	α	α_h	$\alpha_i = 9$ if i is odd
9	α_ℓ	α_h	α_k	
10	β_h	β_k	β_ℓ	
11	β_k	β_ℓ	β_h	$\beta_j = 8$ if cos $2\pi jx$
12	β_ℓ	β_h	β_k	$\beta_j = 9$ if sin $2\pi jx$
13-18	Fourier coef A; xxxx.xx			Sign is overpunched in col. 18
41-50	10 1009 1030			x = -.
51-60	69 0959 1031			These orders are used in the program. They must be punched into the first sum detail cards only if multiple coefficient cards are to be punched.
61-70	23 0977 1343			
71-80	65 0000 1010			

Table 17. Multiple coefficient output cards

Card col.	Contents 2nd sum	3rd sum	Comments
1-2	ℓ	x	x switch expands col. 1-2 y switch expands col. 3-4
3-4	x	y	z switch expands card line
5	x or no x	x or no x	no x first range x second range
6	C_ℓ	C_h	C = 1 for E.C. 2 for O.C. C = 3 for E.S. 4 for O.S. D = blank for O.S. 8 for E.S. D = x for O.C. x/8 for E.C.
7	C_h	C_k	
8	D_k	D_ℓ	
10	sign of value in 69-74		
11	sign of value in 75-80		
15-20	y = 0,11	z = 0,11	
21-26	y = 1,12	z = 1,12	
.	.	.	The second value is for the second range
.	.	.	
.	.	.	
.	.	.	
69-74	y = 9,20	z = 9,20	
75-80	y = 10,-	z = 10,-	

2. Assembly of program deck

To place the program in operation, set the console switches for normal operation with error switches set to stop. The storage entry switches are set at 70 0004 xxxx.

Computer reset and program start will start the loading of the program deck and detail cards. The program deck is made up in the following order:

(a) Drum clear and four-order load routine,
(This consists of five load cards which must be kept in order.),

(b) Program deck,
(This deck also contains the orders for single point punching and 1/80 interval. These are four-order type load cards.),

(c) Sine and cosine decks for the desired interval,
(These are four-order type load cards.),

(d) Calculate by 1/40 (one control card),
(This is four-order type load card and is used only if 1/40 intervals are desired.),

(e) Transfer card,
(This card transfers to the read instruction at 0050 of 70 0951 0048.),

(f) Modification cards for type of punching desired,

(g) Detail cards,
(The input detail cards must be sorted on constant indices and then be sorted into subseries.),

(h) Last card,
(The program punches on a change of index. The last card furnishes such a change so that the last set of sums may be punched. It corresponds to a detail card with zero indices and calls for a sin sin sin product. This leaves the work cells set at zero. The program register will contain the RD instruction at 0300 RD 70 0951 0098.).

In order to rerun for the next sum the storage entry switches should be reset to 00 0000 0050. Pressing computer reset will transfer control to the read instruction at 0050.

The cards in items f, g and h are then run through the machine. The cards in items a, b, c, d and e are used only to put the program on the drum.

3. Tabulation

The final output cards are sorted on columns 4 through 1 and then sorted into two ranges by sorting on column 5. These cards are then tabulated. The tabulator sheet of paper is printed in the same format no matter what the setting of the three translation switches may be. At the left hand side, the contents of columns 1-4 are printed. The third coordinate of the point is implied in the position of the column containing the value of the Fourier series for that point. These columns are labeled, from left to right, by 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 for the first range. The second range results are tabulated below the first range results. The columns in the second range are labeled, from left to right, by 11, 12, 13, 14, 15, 16, 17, 18, 19, 20. The coordinates for points using various translations are obtained in the manner previously discussed.

4. Empty drum cells

The following locations are not used in this program:

1950	1995	1648
0896	1348	1698
0946	1398	1748
1795	1448	1798

1845	1498	1848
1895	1548	1898
1945	1598	1948
		1998.

5. Control card formats

The drum zero card and the four-order loading routine are given in Table 18.

A card punched with

69 0952 0953 45 1444 0954 24 1150 0950 69 0955 0956
45 1444 0048 24 1150 0050 00 0000 0000 00 0000 0000

in columns 1 through 80 will zero the work cells used in storing intermediate sums. This card is not used in ordinary operation.

The calculate by 1/40 control card is a load card punched from column 1 to 80 with

24 1490 1645 20 1496 0300 24 1017 1695 00 0000 1034
24 0490 1745 21 1496 0300 24 0491 0985 21 1497 0300 .

The various punch control cards for multiple coefficient output are listed below.

(a) Punch two ranges and both even and odd index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 1195 0955
24 1942 0956 69 1245 0957 24 1992 0050 00 0000 0000

(b) Punch two ranges and only even index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 1195 0955

24 1942 0956 69 1295 0957 24 1992 0050 00 0000 0000

(c) Punch one range and both even and odd index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 0955 0956

71 0977 0650 24 1942 0050 00 0000 0000 00 0000 0000

(d) Punch one range and only even index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 0955 0956

71 0977 0796 24 1942 0050 00 0000 0000 00 0000 0000

(e) Punch single coefficient cards. These are used if it is desired to return to single coefficient output after switching to multiple coefficient output has been used. There are three cards required.

Card 1 is

69 0952 0953 44 0194 0149 24 0973 0954 69 0955 0956

10 1009 1030 24 0979 0050 00 0000 0000 00 0000 0000 .

Card 2 is

69 0952 0953 69 0959 1031 24 0980 0954 69 0955 0956

23 0977 1343 24 0981 0050 00 0000 0000 00 0000 0000 .

Card 3 is

69 0952 0953 65 0000 1010 24 0982 0050 00 0000 0000

00 0000 0000 00 0000 0000 00 0000 0000 00 0000 0000 .

The transfer from four-order load routine card is a non-load card punched with a zero in each column.

Table 18. Drum zero and four-order load routine

Field	Operation code	Address Data	Address Instruction	Remarks
1	00	0001	0000	
2	00	0000	0000	
3	10	0001	8003	
4	61	0008	0007	drum zero
5	24	0000	8003	
6	70	0004	0004	(1)
7	69	0006	0005	
8	20	1999	0003	
1	69	0002	0003	
2	69	0952	0951	load load routine
3	24	1595	0000	
4	69	0005	0006	
5	70	0984	0050	(2)
6	24	0985	0001	
7	00	0000	0000	
8	00	0000	0000	
1	69	0002	0003	
2	69	0956	0955	
3	24	1695	0000	
4	69	0005	0006	(3)
5	69	0954	0953	
6	24	1645	0001	
7	00	0000	0000	
8	00	0000	0000	
1	69	0002	0003	
2	65	0951	1545	
3	24	0984	0000	
4	69	0005	0006	(4)
5	69	0958	0957	
6	24	1745	0001	
7	00	0000	0000	
8	00	0000	0000	
1	00	0000	0000	
2	00	0000	0000	
3	00	0000	0000	(5)
4	69	0005	0006	
5	45	1595	0952	
6	24	0984	0985	
7	00	0000	0000	
8	00	0000	0000	

6. The program deck

The cards in the program deck are listed in Table 19 with the contents of each card displayed on one line. The trigonometric decks for 1/40 interval are listed in Table 20. The 1/80 interval decks are listed in Table 21. These addresses and orders must be made into four-order load cards.

TABLE 19. PROGRAM ORDERS FOR T.D.F. 40-80 (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
01946902470 20¤		0247000000008¤		0200240986080¤		0800650978189C	
1893940596029H		0298160444059F		0444000000100¤		0596200978049D	
0494690047085¤		0047440348094I		0850241044054D		0544650447090¤	
0447100996049E		0900210984059D		0594118001800B		0495440899134E	
0899460644084D		0644110497069D		0497000000000A		0694210985074D	
0744118001079D		0794100497054E		0844210985089D		0894118001054E	
0545710977094D		0944100984099D		0994110547104D		0547000020000¤	
0348108001039H		0398100645099I		0999151094090¤		1094000050000¤	
0949691144059G		1144440348095¤		0597241044064G		0647650978119D	
1194150697124D		0697000000100¤		1244200978129D		1294650747090¤	
0747100997049E		0950651344800B		1344210996100¤		1000161943079G	
1943211996100¤		0797451050139D		1050151993800B		1993212046100¤	
1394650847800B		0847210997110¤		1100161494115¤		1494211997110¤	
1444150897800B		0897212047110¤		1200650977144B		1442698003024H	
0248230954149B		1492300002034I		0349158001154B		1542350006159B	
1592150978159D		1642940399029G		0297160245039I		0245000000100¤	
0399200986059E		0595691544039G		1544230978040¤		0397240350034G	
0347650550103B		0550690996800C		1032101036800B		1036240977099A	
0991110044044I		0044240985099A		0449440955144E		1009240986099A	
1030151035800B		1035000050000¤		1031221037800A		1010690977169C	
1693300004095G		1343300004139C		1393350002049I		0499461742179B	
1742160295054I		0295000000000H		1792150345054I		0345000000000I	
0549690978035¤		0400651037009F		0096150599800B		0599000050003H	
1048690979144C		1443300004014F		0146230979149C		1493300004154C	
1543350002064I		0649461842189B		1842160295069I		1892150345069I	
0699690980024F		0246230980189D		0600660986029F		0296200986159C	
1593690346074I		0346230978169B		0749240350164C		1643650396024D	
0396000550000¤		0244150550103B		1692658003079I		0799690979029D	
0294230979034D		0344690980039D		0394230980094H		0650670986174C	
0446151500074F		1500000000100¤		0849200986179C		1793690496039E	
0496230978040¤		0395240350184C		1843650546044E		0546690997800C	
0445200550103B		0050700951004H		0300700951009H		0971210977009E	
0095690958096I		0969240978014I		0098600952096E		0965110968097C	
0973440194014I		0149600951100E		1005690958101A		1011450964004F	
0046910099030¤		0099650960096F		0966201025098G		0987150996097D	
0974200996104I		1049651025104A		1041151046104¤		1040201046109I	
1099651025109A		1091151096109¤		1090201096114I		1149651025114A	
1141151146114¤		1140201146119I		1199651025119A		1191151196119¤	
1190201196124I		1249651025124A		1241151246124¤		1240201246129I	
1299651025129A		1291151296129¤		1290201296134I		1349651025134A	
1341151346134¤		1340201346139I		1399651025139A		1391151396139¤	
1390201396144I		1449651025144A		1441151446144¤		1440201446149I	
1499651025149A		1491151496149¤		1490201496154I		1549651025154A	
1541151546154¤		1540201546159I		1599651025159A		1591151596159¤	

TABLE 19. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1590201596164I		1649651025164A		1641151646164¤		1640201646169I	
1699651025169A		1691151696169¤		1690201696174I		1749651025174A	
1741151746174¤		1740201746179I		1799651025179A		1791151796179¤	
1790201796184I		1849651025184A		1841151846184¤		1840201846189I	
1899651025189A		1891151896189¤		1890201896194I		1949651025194A	
1941151946194¤		1940201946199I		1999651025199A		1991151996199¤	
1990201996030¤		0964910967101I		0967941020102B		10206680031026	
1027150094019I		0094190040004B		0199201015097F		0976201037109C	
1093650996100B		1002150960103I		1039200996029I		0299600951100F	
1006100963101G		0963000001000¤		1022668003099¤		0990150993009G	
0993190040004C		0097201015097E		0975201037014D		0144650997100C	
1003150960098H		0988200997015¤		0150600953100H		1008100963101G	
1019941023102F		1023668003098I		0989151043019H		1043191090004B	
0198201015102D		1024201037014G		0147600951101G		1026668003104B	
1042150145024I		0145191090004C		0249201015102A		1021201037019G	
0197600951101G		1017191028101C		1028000000002E		1013300002102I	
1029691033103H		1033000000000¤		1038231092019E		0195658001100D	
1004300001800B		0000000000103D		0500000000103D		0250690958101F	
0750690958101H		1016941143119C		1018941243129C		1143651996114B	
1193651997119B		1243651996124B		1293651997129B		1142150960134B	
1192150960139B		1242160960134B		1292160960139B		1342201996103D	
1392201997103D		1034651037099B		0992150045004I		0045000050005¤	
0049200954100G		1007600960101E		0092101096009¤		0142101146014¤	
0192101196019¤		0242101246024¤		0292101296029¤		0342101346034¤	
0392101396039¤		0442101446044¤		0492101496049¤		0542101546054¤	
0592101596059¤		0642101646064¤		0692101696069¤		0742101746074¤	
0792101796079¤		0842101846084¤		0892101896089¤		0942101946094¤	
0043101047004A		0093101097009A		0143101147014A		0193101197019A	
0243101247024A		0293101297029A		0343101347034A		0393101397039A	
0443101447044A		0493101497049A		0543101547054A		0593101597059A	
0643101647064A		0693101697069A		0743101747074A		0793101797079A	
0843101847084A		0893101897089A		0943101947094A		0940211946030¤	
0041211047100A		0091211097100A		0141211147100A		0191211197100A	
0641211647100A		0691211697100A		0741211747100A		0791211797100A	
0441211447100A		0491211497100A		0541211547100A		0591211597100A	
0241211247100A		0291211297100A		0341211347100A		0391211397100A	
0841211847100A		0891211897100A		0941211947030¤		0645000001000¤	
1594920947125¤		0947951644049H		1644160448130¤		0448000008007¤	
0498160695130¤		0695000009006¤		1250951694054H		1694160598130¤	
0598000008006¤		0745000009005¤		1300698002174D		1744930148135¤	
0148961794019F		1794160648101B		0648000080070¤		0196161400101B	
1350961844064F		1400000090060¤		1844160698101B		0698000080060¤	
0646161450101B		1450000090050¤		1894910748155¤		0748650986079E	
0948650978104E		1045910998170¤		0998650986194D		1944961992175¤	
0945000080000¤		1600150995165¤		0995000090000¤		1650200986194B	

TABLE 19. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0848000009000¤		0696690978089E		0895910898160¤		0898150945165¤	
0795150798069F		0798000008000¤		1550650986084E		0845150848069F	
1750151098199B		1098000010000¤		1700650986109E		1095961148149E	
1148161098149E		0746698002199D		1994961198180¤		1198160945185¤	
1800160995185¤		1850698002114E		1145951248190¤		1248160798084I	
1900160848084I		1012698002164B		1150451444004H		0048600952096B	
0962210968097A		0042101046004¤		1001650954096A		0961201015097B	
0972201037099B		0040211046100A		0090211096100A		0140211146100A	
0190211196100A		0240211246100A		0290211296100A		0340211346100A	
0390211396100A		0440211446100A		0490211496100A		0540211546100A	
0590211596100A		0640211646100A		0690211696100A		0740211746100A	
0790211796100A		0840211846100A		0890211896100A		0796690970084F	
0548160745130¤		1743940446079F		0846240550095¤		0970690996800C	
0978000088888H		0979101009103¤		0980690959103A		0981230977134C	
0982650000101¤		1495200986199B		1345461395094D		1395100497094D	
1195710977060¤		1245710977065¤		1295710977079F		1298000050000¤	
1445151298095F		1245710977065¤		1295710977079F		1298000050000¤	
1750151098149E		1495200986199B					

TABLE 20. SINE AND COSINE TABLE BY 1/40 INTERVAL (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1051156434000*		1052309017000*		1053453990000*		1054587785000*	
1055707107000*		1056809017000*		1057891007000*		1058951057000*	
1059987688000*		1060999999000*		1061987688000*		1062951057000*	
1063891007000*		1064809017000*		1065707107000*		1066587785000*	
1067453990000*		1068309017000*		1069156434000*		1070000000000*	
1071156434000¤		1072309017000¤		1073453990000¤		1074587785000¤	
1075707107000¤		1076809017000¤		1077891007000¤		1078951057000¤	
1079987688000¤		1080999999000¤		1081987688000¤		1082951057000¤	
1083891007000¤		1084809017000¤		1085707107000¤		1086587785000¤	
1087453990000¤		1088309017000¤		1089156434000¤		1101309017000*	
1102587785000*		1103809017000*		1104951057000*		1105999999000*	
1106951057000*		1107809017000*		1108587785000*		1109309017000*	
1110000000000*		1111309017000¤		1112587785000¤		1113809017000¤	
1114951057000¤		1115999999000¤		1116951057000¤		1117809017000¤	
1118587785000¤		1119309017000¤		1120000000000¤		1121309017000*	
1122587785000*		1123809017000*		1124951057000*		1125999999000*	
1126951057000*		1127809017000*		1128587785000*		1129309017000*	
1130000000000*		1131309017000¤		1132587785000¤		1133809017000¤	
1134951057000¤		1135999999000¤		1136951057000¤		1137809017000¤	
1138587785000¤		1139309017000¤		1151453990000*		1152809017000*	
1153987688000*		1154951057000*		1155707107000*		1156309017000*	
1157156434000¤		1158587785000¤		1159891007000¤		1160999999000¤	
1161891007000¤		1162587785000¤		1163156434000¤		1164309017000*	
1165707107000*		1166951057000*		1167987688000*		1168809017000*	
1169453990000*		1170000000000*		1171453990000¤		1172809017000¤	
1173987688000¤		1174951057000¤		1175707107000¤		1176309017000¤	
1177156434000*		1178587785000*		1179891007000*		1180999999000*	
1181891007000*		1182587785000*		1183156434000*		1184309017000¤	
1185707107000¤		1186951057000¤		1187987688000¤		1188809017000¤	
1189453990000¤		1201587785000*		1202951057000*		1203951057000*	
1204587785000*		1205000000000*		1206587785000¤		1207951057000¤	
1208951057000¤		1209587785000¤		1210000000000¤		1211587785000*	
1212951057000*		1213951057000*		1214587785000*		1215000000000*	
1216587785000¤		1217951057000¤		1218951057000¤		1219587785000¤	
1220000000000¤		1221587785000*		1222951057000*		1223951057000*	
1224587785000*		1225000000000*		1226587785000¤		1227951057000¤	
1228951057000¤		1229587785000¤		1230000000000¤		1231587785000*	
1232951057000*		1233951057000*		1234587785000*		1235000000000*	
1236587785000¤		1237951057000¤		1238951057000¤		1239587785000¤	
1251707107000*		1252999999000*		1253707107000*		1254000000000*	
1255707107000¤		1256999999000¤		1257707107000¤		1258000000000¤	
1259707107000*		1260999999000*		1261707107000*		1262000000000*	
1263707107000¤		1264999999000¤		1265707107000¤		1266000000000¤	
1267707107000*		1268999999000*		1269707107000*		1270000000000*	

TABLE 20. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1271707107000¤		1272999999000¤		1273707107000¤		1274000000000¤	
1275707107000*		1276999999000*		1277707107000*		1278000000000*	
1279707107000¤		1280999999000¤		1281707107000¤		1282000000000¤	
1283707107000*		1284999999000*		1285707107000*		1286000000000*	
1287707107000¤		1288999999000¤		1289707107000¤		1301809017000*	
1302951057000*		1303309017000*		1304587785000¤		1305999999000¤	
1306587785000¤		1307309017000*		1308951057000*		1309809017000*	
1310000000000*		1311809017000¤		1312951057000¤		1313309017000¤	
1314587785000*		1315999999000*		1316587785000*		1317309017000¤	
1318951057000¤		1319809017000¤		1320000000000¤		1321809017000*	
1322951057000*		1323309017000*		1324587785000¤		1325999999000¤	
1326587785000¤		1327309017000*		1328951057000*		1329809017000*	
1330000000000*		1331809017000¤		1332951057000¤		1333309017000¤	
1334587785000*		1335999999000*		1336587785000*		1337309017000¤	
1338951057000¤		1339809017000¤		1351891007000*		1352809017000*	
1353156434000¤		1354951057000¤		1355707107000¤		1356309017000*	
1357987688000*		1358587785000*		1359453990000¤		1360999999000¤	
1361453990000¤		1362587785000*		1363987688000*		1364309017000*	
1365707107000¤		1366951057000¤		1367156434000¤		1368809017000*	
1369891007000*		1370000000000*		1371891007000¤		1372809017000¤	
1373156434000*		1374951057000*		1375707107000*		1376309017000¤	
1377987688000¤		1378587785000¤		1379453990000*		1380999999000*	
1381453990000*		1382587785000¤		1383987688000¤		1384309017000¤	
1385707107000*		1386951057000*		1387156434000*		1388809017000¤	
1389891007000¤		1401951057000*		1402587785000*		1403587785000¤	
1404951057000¤		1405000000000¤		1406951057000*		1407587785000*	
1408587785000¤		1409951057000¤		1410000000000¤		1411951057000*	
1412587785000*		1413587785000¤		1414951057000¤		1415000000000¤	
1416951057000*		1417587785000*		1418587785000¤		1419951057000¤	
1420000000000¤		1421951057000*		1422587785000*		1423587785000¤	
1424951057000¤		1425000000000¤		1426951057000*		1427587785000*	
1428587785000¤		1429951057000¤		1430000000000¤		1431951057000*	
1432587785000*		1433587785000¤		1434951057000¤		1435000000000¤	
1436951057000*		1437587785000*		1438587785000¤		1439951057000¤	
1451987688000*		1452309017000*		1453891007000¤		1454587785000¤	
1455707107000*		1456809017000*		1457453990000¤		1458951057000¤	
1459156434000*		1460999999000*		1461156434000*		1462951057000¤	
1463453990000¤		1464809017000*		1465707107000*		1466587785000¤	
1467891007000¤		1468309017000*		1469987688000*		1470000000000*	
1471987688000¤		1472309017000¤		1473891007000*		1474587785000*	
1475707107000¤		1476809017000¤		1477453990000*		1478951057000*	
1479156434000¤		1480999999000¤		1481156434000¤		1482951057000*	
1483453990000*		1484809017000¤		1485707107000¤		1486587785000*	
1487891007000*		1488309017000¤		1489987688000¤		1501999999000*	
1502000000000*		1503999999000¤		1504000000000¤		1505999999000*	

TABLE 20. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1506000000000*		1507999999000¤		1508000000000¤		1509999999000*	
1510000000000*		1511999999000¤		1512000000000¤		1513999999000*	
1514000000000*		1515999999000¤		1516000000000¤		1517999999000*	
1518000000000*		1519999999000¤		1520000000000¤		1521999999000*	
1522000000000*		1523999999000¤		1524000000000¤		1525999999000*	
1526000000000*		1527999999000¤		1528000000000¤		1529999999000*	
1530000000000*		1531999999000¤		1532000000000¤		1533999999000*	
1534000000000*		1535999999000¤		1536000000000¤		1537999999000*	
1538000000000*		1539999999000¤		1536000000000¤		1537999999000*	
0001987688000¤		0002951057000¤		0003891007000¤		0004809017000¤	
0005707107000¤		0006587785000¤		0007453990000¤		0008309017000¤	
0009156434000¤		0010000000000¤		0011156434000*		0012309017000*	
0013453990000*		0014587785000*		0015707107000*		0016809017000*	
0017891007000*		0018951057000*		0019987688000*		0020999999000*	
0021987688000*		0022951057000*		0023891007000*		0024809017000*	
0025707107000*		0026587785000*		0027453990000*		0028309017000*	
0029156434000*		0030000000000*		0031156434000¤		0032309017000¤	
0033453990000¤		0034587785000¤		0035707107000¤		0036809017000¤	
0037891007000¤		0038951057000¤		0039987688000¤		0051951057000¤	
0052809017000¤		0053587785000¤		0054309017000¤		0055000000000¤	
0056309017000*		0057587785000*		0058809017000*		0059951057000*	
0060999999000*		0061951057000*		0062809017000*		0063587785000*	
0064309017000*		0065000000000*		0066309017000¤		0067587785000¤	
0068809017000¤		0078809017000*		0069951057000¤		0070999999000¤	
0071951057000¤		0072809017000¤		0073587785000¤		0074309017000¤	
0075000000000¤		0076309017000*		0077587785000*		0079951057000*	
0080999999000*		0081951057000*		0082809017000*		0083587785000*	
0084309017000*		0085000000000*		0086309017000¤		0087587785000¤	
0088809017000¤		0089951057000¤		0101891007000¤		0102587785000¤	
0103156434000¤		0104309017000*		0105707107000*		0106951057000*	
0107987688000*		0108809017000*		0109453990000*		0110000000000*	
0111453990000¤		0112809017000¤		0113987688000¤		0114951057000¤	
0115707107000¤		0116309017000¤		0117156434000*		0118587785000*	
0119891007000*		0120999999000*		0121891007000*		0122587785000*	
0123156434000*		0124309017000¤		0125707107000¤		0126951057000¤	
0127987688000¤		0128809017000¤		0129453990000¤		0130000000000¤	
0131453990000*		0132809017000*		0133987688000*		0134951057000*	
0135707107000*		0136309017000*		0137156434000¤		0138587785000¤	
0139891007000¤		0151809017000¤		0152309017000¤		0153309017000*	
0154809017000*		0155999999000*		0156809017000*		0157309017000*	
0158309017000¤		0159809017000¤		0160999999000¤		0161809017000¤	
0162309017000¤		0163309017000*		0164809017000*		0165999999000*	
0166809017000*		0167309017000*		0168309017000¤		0169809017000¤	
0170999999000¤		0171809017000¤		0172309017000¤		0173309017000*	
0174809017000*		0175999999000*		0176809017000*		0177309017000*	

TABLE 20. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0178309017000¤		0179809017000¤		0180999999000¤		0181809017000¤	
0182309017000¤		0183309017000*		0184809017000*		0185999999000*	
0186809017000*		0187309017000*		0188309017000¤		0189809017000¤	
0201707107000¤		0202000000000¤		0203707107000*		0204999999000*	
0205707107000*		0206000000000*		0207707107000¤		0208999999000¤	
0209707107000¤		0210000000000¤		0211707107000*		0212999999000*	
0213707107000*		0214000000000*		0215707107000¤		0216999999000¤	
0217707107000¤		0218000000000¤		0219707107000*		0220999999000*	
0221707107000*		0222000000000*		0223707107000¤		0224999999000¤	
0225707107000¤		0226000000000¤		0227707107000*		0228999999000*	
0229707107000*		0230000000000*		0231707107000¤		0232999999000¤	
0233707107000¤		0234000000000¤		0235707107000*		0236999999000*	
0237707107000*		0238000000000*		0239707107000¤		0251587785000¤	
0252309017000*		0253951057000*		0254809017000*		0255000000000*	
0256809017000¤		0257951057000¤		0258309017000¤		0259587785000*	
0260999999000*		0261587785000*		0262309017000¤		0263951057000¤	
0264809017000¤		0265000000000¤		0266809017000*		0267951057000*	
0268309017000*		0269587785000¤		0270999999000¤		0271587785000¤	
0272309017000*		0273951057000*		0274809017000*		0275000000000*	
0276809017000¤		0277951057000¤		0278309017000¤		0279587785000*	
0280999999000*		0281587785000*		0282309017000¤		0283951057000¤	
0284809017000¤		0285000000000¤		0286809017000*		0287951057000*	
0288309017000*		0289587785000¤		0301453990000¤		0302587785000*	
0303987688000*		0304309017000*		0305707107000¤		0306951057000¤	
0307156434000¤		0308809017000*		0309891007000*		0310000000000*	
0311891007000¤		0312809017000¤		0313156434000*		0314951057000*	
0315707107000*		0316309017000¤		0317987688000¤		0318587785000¤	
0319453990000*		0320999999000*		0321453990000*		0322587785000¤	
0323987688000¤		0324309017000¤		0325707107000*		0326951057000*	
0327156434000*		0328809017000¤		0329891007000¤		0330000000000¤	
0331891007000*		0332809017000*		0333156434000¤		0334951057000¤	
0335707107000¤		0336309017000*		0337987688000*		0338587785000*	
0339453990000¤		0351309017000¤		0352809017000*		0353809017000*	
0354309017000¤		0355999999000¤		0356309017000¤		0357809017000*	
0358809017000*		0359309017000¤		0360999999000¤		0361309017000¤	
0362809017000*		0363809017000*		0364309017000¤		0365999999000¤	
0366309017000¤		0367809017000*		0369309017000¤		0370999999000¤	
0371309017000¤		0372809017000*		0373809017000*		0374309017000¤	
0375999999000¤		0376309017000¤		0377809017000*		0368809017000*	
0378809017000*		0379309017000¤		0380999999000¤		0381309017000¤	
0382809017000*		0383809017000*		0384309017000¤		0385999999000¤	
0386309017000¤		0387809017000*		0388809017000*		0389309017000¤	
0401156434000¤		0402951057000*		0403453990000*		0404809017000¤	
0405707107000¤		0406587785000*		0407891007000*		0408309017000¤	
0409987688000¤		0410000000000¤		0411987688000*		0412309017000*	

TABLE 20. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0413891007000□		0414587785000□		0415707107000*		0416809017000*	
0417453990000□		0418951057000□		0419156434000*		0420999999000*	
0421156434000*		0422951057000□		0423453990000□		0424809017000*	
0425707107000*		0426587785000□		0427891007000□		0428309017000*	
0429987688000*		0430000000000*		0431987688000□		0432309017000□	
0433891007000*		0434587785000*		0435707107000□		0436809017000□	
0437453990000*		0438951057000*		0439156434000□		0451000000000□	
0452999999000*		0453000000000*		0454999999000□		0455000000000□	
0456999999000*		0457000000000*		0458999999000□		0459000000000□	
0460999999000*		0461000000000*		0462999999000□		0463000000000□	
0464999999000*		0465000000000*		0466999999000□		0467000000000□	
0468999999000*		0469000000000*		0470999999000□		0471000000000□	
0472999999000*		0473000000000*		0474999999000□		0475000000000□	
0476999999000*		0477000000000*		0478999999000□		0479000000000□	
0480999999000*		0481000000000*		0482999999000□		0483000000000□	
0484999999000*		0485000000000*		0486999999000□		0487000000000□	
0488999999000*		0489000000000*		0486999999000□		0487000000000□	

TABLE 21. SINE AND COSINE TABLE BY 1/80 INTERVAL (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1089078459000¤		1139156434000¤		1189233445000¤		1239309017000¤	
1289382683000¤		1339453990000¤		1389522499000¤		1439587785000¤	
1489649448000¤		1539707107000¤		1589760406000¤		1639809017000¤	
1689852640000¤		1739891007000¤		1789923880000¤		1839951057000¤	
1889972370000¤		1939987688000¤		1989996917000¤		1088156434000¤	
1138309017000¤		1188453990000¤		1238587785000¤		1288707107000¤	
1338809017000¤		1388891007000¤		1438951057000¤		1488987688000¤	
1538999999000¤		1588987688000¤		1638951057000¤		1688891007000¤	
1738809017000¤		1788707107000¤		1838587785000¤		1888453990000¤	
1938309017000¤		1988156434000¤		1087233445000¤		1137453990000¤	
1187649448000¤		1237809017000¤		1287923880000¤		1337987688000¤	
1387996917000¤		1437951057000¤		1487852640000¤		1537707107000¤	
1587522499000¤		1637309017000¤		1687078459000¤		1737156434000*	
1787382683000*		1837587785000*		1887760406000*		1937891007000*	
1987972370000*		1086309017000¤		1136587785000¤		1186809017000¤	
1236951057000¤		1286999999000¤		1336951057000¤		1386809017000¤	
1436587785000¤		1486309017000¤		1536000000000*		1586309017000*	
1636587785000*		1686809017000*		1736951057000*		1786999999000*	
1836951057000*		1886809017000*		1936587785000*		1986309017000*	
1085382683000¤		1135707107000¤		1185923880000¤		1235999999000¤	
1285923880000¤		1335707107000¤		1385382683000¤		1435000000000*	
1485382683000*		1535707107000*		1585923880000*		1635999999000*	
1685923880000*		1735707107000*		1785382683000*		1835000000000¤	
1885382683000¤		1935707107000¤		1985923880000¤		1084453990000¤	
1134809017000¤		1184987688000¤		1234951057000¤		1284707107000¤	
1334309017000¤		1384156434000*		1434587785000*		1484891007000*	
1534999999000*		1584891007000*		1634587785000*		1684156434000*	
1734309017000¤		1784707107000¤		1834951057000¤		1884987688000¤	
1934809017000¤		1984453990000¤		1083522499000¤		1133891007000¤	
1183996917000¤		1233809017000¤		1283382683000¤		1333156434000*	
1383649448000*		1433951057000*		1483972370000*		1533707107000*	
1583233445000*		1633309017000¤		1683760406000¤		1733987688000¤	
1783923880000¤		1833587785000¤		1883078459000¤		1933453990000*	
1983852640000*		1082587785000¤		1132951057000¤		1182951057000¤	
1232587785000¤		1282000000000*		1332587785000*		1382951057000*	
1432951057000*		1482587785000*		1532000000000¤		1582587785000¤	
1632951057000¤		1682951057000¤		1732587785000¤		1782000000000*	
1832587785000*		1882951057000*		1932951057000*		1982587785000*	
1081649448000¤		1131987688000¤		1181852640000¤		1231309017000¤	
1281382683000*		1331891007000*		1381972370000*		1431587785000*	
1481078459000¤		1531707107000¤		1581996917000¤		1631809017000¤	
1681233445000¤		1731453990000*		1781923880000*		1831951057000*	
1881522499000*		1931156434000¤		1981760406000¤		1080707107000¤	
1130999999000¤		1180707107000¤		1230000000000*		1280707107000*	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1330999999000*		1380707107000*		1430000000000¤		1480707107000¤	
1530999999000¤		1580707107000¤		1630000000000*		1680707107000*	
1730999999000*		1780707107000*		1830000000000¤		1880707107000¤	
1930999999000¤		1980707107000¤		1079760406000¤		1129987688000¤	
1179522499000¤		1229309017000*		1279923880000*		1329891007000*	
1379233445000*		1429587785000¤		1479996917000¤		1529707107000¤	
1579078459000*		1629809017000*		1679972370000*		1729453990000*	
1779382683000¤		1829951057000¤		1879852640000¤		1929156434000¤	
1979649448000*		1078809017000¤		1128951057000¤		1178309017000¤	
1228587785000*		1278999999000*		1328587785000*		1378309017000¤	
1428951057000¤		1478809017000¤		1528000000000*		1578809017000*	
1628951057000*		1678309017000*		1728587785000¤		1778999999000¤	
1828587785000¤		1878309017000*		1928951057000*		1978809017000*	
1077852640000¤		1127891007000¤		1177078459000¤		1227809017000*	
1277923880000*		1327156434000*		1377760406000¤		1427951057000¤	
1477233445000¤		1527707107000*		1577972370000*		1627309017000*	
1677649448000¤		1727987688000¤		1777382683000¤		1827587785000*	
1877996917000*		1927453990000*		1977522499000¤		1076891007000¤	
1126809017000¤		1176156434000*		1226951057000*		1276707107000*	
1326309017000¤		1376987688000¤		1426587785000¤		1476453990000*	
1526999999000*		1576453990000*		1626587785000¤		1676987688000¤	
1726309017000¤		1776707107000*		1826951057000*		1876156434000*	
1926809017000¤		1976891007000¤		1075923880000¤		1125707107000¤	
1175382683000*		1225999999000*		1275382683000*		1325707107000¤	
1375923880000¤		1425000000000*		1475923880000*		1525707107000*	
1575382683000¤		1625999999000¤		1675382683000¤		1725707107000*	
1775923880000*		1825000000000¤		1875923880000¤		1925707107000¤	
1975382683000*		1074951057000¤		1124587785000¤		1174587785000*	
1224951057000*		1274000000000¤		1324951057000¤		1374587785000¤	
1424587785000*		1474951057000*		1524000000000¤		1574951057000¤	
1624587785000¤		1674587785000*		1724951057000*		1774000000000¤	
1824951057000¤		1874587785000¤		1924587785000*		1974951057000*	
1073972370000¤		1123453990000¤		1173760406000*		1223809017000*	
1273382683000¤		1323987688000¤		1373078459000¤		1423951057000*	
1473522499000*		1523707107000¤		1573852640000¤		1623309017000*	
1673996917000*		1723156434000*		1773923880000¤		1823587785000¤	
1873649448000*		1923891007000*		1973233445000¤		1072987688000¤	
1122309017000¤		1172891007000*		1222587785000*		1272707107000¤	
1322809017000¤		1372453990000*		1422951057000*		1472156434000¤	
1522999999000¤		1572156434000¤		1622951057000*		1672453990000*	
1722809017000¤		1772707107000¤		1822587785000*		1872891007000*	
1922309017000¤		1972987688000¤		1071996917000¤		1121156434000¤	
1171972370000*		1221309017000*		1271923880000¤		1321453990000¤	
1371852640000*		1421587785000*		1471760406000¤		1521707107000¤	
1571649448000*		1621809017000*		1671522499000¤		1721891007000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1771382683000*		1821951057000*		1871233445000¤		1921987688000¤	
1971078459000*		1070999999000¤		1120000000000*		1170999999000*	
1220000000000¤		1270999999000¤		1320000000000*		1370999999000*	
1420000000000¤		1470999999000¤		1520000000000*		1570999999000*	
1620000000000¤		1670999999000¤		1720000000000*		1770999999000*	
1820000000000¤		1870999999000¤		1920000000000*		1970999999000*	
1069996917000¤		1119156434000*		1169972370000*		1219309017000¤	
1269923880000¤		1319453990000*		1369852640000*		1419587785000¤	
1469760406000¤		1519707107000*		1569649448000*		1619809017000¤	
1669522499000¤		1719891007000*		1769382683000*		1819951057000¤	
1869233445000¤		1919987688000*		1969078459000*		1068987688000¤	
1118309017000*		1168891007000*		1218587785000¤		1268707107000¤	
1318809017000*		1368453990000*		1418951057000¤		1468156434000¤	
1518999999000*		1568156434000¤		1618951057000¤		1668453990000*	
1718809017000*		1768707107000¤		1818587785000¤		1868891007000*	
1918309017000*		1968987688000¤		1067972370000¤		1117453990000*	
1167760406000*		1217809017000¤		1267382683000¤		1317987688000*	
1367078459000¤		1417951057000¤		1467522499000*		1517707107000*	
1567852640000¤		1617309017000¤		1667996917000*		1717156434000¤	
1767923880000¤		1817587785000*		1867649448000*		1917891007000¤	
1967233445000¤		1066951057000¤		1116587785000*		1166587785000*	
1216951057000¤		1266000000000*		1316951057000*		1366587785000¤	
1416587785000¤		1466951057000*		1516000000000¤		1566951057000¤	
1616587785000*		1666587785000*		1716951057000¤		1766000000000*	
1816951057000*		1866587785000¤		1916587785000¤		1966951057000*	
1065923880000¤		1115707107000*		1165382683000*		1215999999000¤	
1265382683000*		1315707107000*		1365923880000¤		1415000000000*	
1465923880000*		1515707107000¤		1565382683000¤		1615999999000*	
1314309017000*		1364987688000¤		1414587785000*		1464453990000*	
1114809017000*		1164156434000*		1214951057000¤		1264707107000*	
1865923880000¤		1915707107000*		1965382683000*		1064891007000¤	
1665382683000¤		1715707107000¤		1765923880000*		1815000000000¤	
1514999999000¤		1564453990000*		1614587785000*		1664987688000¤	
1714309017000*		1764707107000*		1814951057000¤		1864156434000*	
1914809017000*		1964891007000¤		1063852640000¤		1113891007000*	
1163078459000¤		1213809017000¤		1263923880000*		1313156434000¤	
1363760406000¤		1413951057000*		1463233445000¤		1513707107000¤	
1563972370000*		1613309017000¤		1663649448000¤		1713987688000*	
1763382683000¤		1813587785000¤		1863996917000*		1913453990000¤	
1963522499000¤		1062809017000¤		1112951057000*		1162309017000¤	
1212587785000¤		1262999999000*		1312587785000¤		1362309017000¤	
1412951057000*		1462809017000¤		1512000000000*		1562809017000*	
1612951057000¤		1662309017000*		1712587785000*		1762999999000¤	
1812587785000*		1862309017000*		1912951057000¤		1962809017000*	
1061760406000¤		1111987688000*		1161522499000¤		1211309017000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1261923880000*		1311891007000¤		1361233445000*		1411587785000*	
1461996917000¤		1511707107000*		1561078459000*		1611809017000¤	
1661972370000*		1711453990000¤		1761382683000¤		1811951057000*	
1861852640000¤		1911156434000*		1961649448000*		1060707107000¤	
1110999999000*		1160707107000¤		1210000000000*		1260707107000*	
1310999999000¤		1360707107000*		1410000000000¤		1460707107000¤	
1510999999000*		1560707107000¤		1610000000000*		1660707107000*	
1710999999000¤		1760707107000*		1810000000000¤		1860707107000¤	
1910999999000*		1960707107000¤		1059649448000¤		1109987688000*	
1159852640000¤		1209309017000*		1259382683000*		1309891007000¤	
1359972370000*		1409587785000¤		1459078459000¤		1509707107000*	
1208587785000*		1258000000000¤		1308587785000¤		1358951057000*	
1959760406000¤		1058587785000¤		1108951057000*		1158951057000¤	
1759923880000*		1809951057000¤		1859522499000*		1909156434000*	
1559996917000¤		1609809017000*		1659233445000¤		1709453990000¤	
1408951057000¤		1458587785000*		1508000000000¤		1558587785000¤	
1608951057000*		1658951057000¤		1708587785000*		1758000000000¤	
1808587785000¤		1858951057000*		1908951057000¤		1958587785000*	
1057522499000¤		1107891007000*		1157996917000¤		1207809017000*	
1257382683000¤		1307156434000¤		1357649448000*		1407951057000¤	
1457972370000*		1507707107000¤		1557233445000*		1607309017000*	
1657760406000¤		1707987688000*		1757923880000¤		1807587785000*	
1857078459000¤		1907453990000¤		1957852640000*		1056453990000¤	
1106809017000*		1156987688000¤		1206951057000*		1256707107000¤	
1306309017000*		1356156434000*		1406587785000¤		1456891007000*	
1506999999000¤		1556891007000*		1606587785000¤		1656156434000*	
1706309017000*		1756707107000¤		1806951057000*		1856987688000¤	
1906809017000*		1956453990000¤		1055382683000¤		1105707107000*	
1155923880000¤		1205999999000*		1255923880000¤		1305707107000*	
1355382683000¤		1405000000000*		1455382683000*		1505707107000¤	
1555923880000*		1605999999000¤		1655923880000*		1705707107000¤	
1755382683000*		1805000000000¤		1855382683000¤		1905707107000*	
1955923880000¤		1054309017000¤		1104587785000*		1154809017000¤	
1204951057000*		1254999999000¤		1304951057000*		1354809017000¤	
1404587785000*		1454309017000¤		1504000000000*		1554309017000*	
1604587785000¤		1654809017000*		1704951057000¤		1754999999000*	
1804951057000¤		1854809017000*		1904587785000¤		1954309017000*	
1053233445000¤		1103453990000*		1153649448000¤		1203809017000*	
1253923880000¤		1303987688000*		1353996917000¤		1403951057000*	
1453852640000¤		1503707107000*		1553522499000¤		1603309017000*	
1653078459000¤		1703156434000¤		1753382683000*		1803587785000¤	
1853760406000*		1903891007000¤		1953972370000*		1052156434000¤	
1102309017000*		1152453990000¤		1202587785000*		1252707107000¤	
1302809017000*		1352891007000¤		1402951057000*		1452987688000¤	
1502999999000*		1552987688000¤		1602951057000*		1652891007000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1702809017000*		1752707107000¤		1802587785000*		1852453990000¤	
1902309017000*		1952156434000¤		1051078459000¤		1101156434000*	
1151233445000¤		1201309017000*		1251382683000¤		1301453990000*	
1351522499000¤		1401587785000*		1451649448000¤		1501707107000*	
1551760406000¤		1601809017000*		1651852640000¤		1701891007000*	
1751923880000¤		1801951057000*		1851972370000¤		1901987688000*	
1951996917000¤		1801951057000*		1851972370000¤		1901987688000*	
0039996917000¤		0089987688000¤		0139972370000¤		0189951057000¤	
0239923880000¤		0289891007000¤		0339852640000¤		0389809017000¤	
0439760406000¤		0489707107000¤		0539649448000¤		0589587785000¤	
0639522499000¤		0689453990000¤		0739382683000¤		0789309017000¤	
0839233445000¤		0889156434000¤		0939078459000¤		0038987688000¤	
0088951057000¤		0138891007000¤		0188809017000¤		0238707107000¤	
0288587785000¤		0338453990000¤		0388309017000¤		0438156434000¤	
0488000000000*		0538156434000*		0588309017000*		0638453990000*	
0688587785000*		0738707107000*		0788809017000*		0838891007000*	
0888951057000*		0938987688000*		0037972370000¤		0087891007000¤	
0137760406000¤		0187587785000¤		0237382683000¤		0287156434000¤	
0337078459000*		0387309017000*		0437522499000*		0487707107000*	
0537852640000*		0587951057000*		0637996917000*		0687987688000*	
0737923880000*		0787809017000*		0837649448000*		0887453990000*	
0937233445000*		0036951057000¤		0086809017000¤		0136587785000¤	
0186309017000¤		0236000000000*		0286309017000*		0336587785000*	
0386809017000*		0436951057000*		0486999999000*		0536951057000*	
0586809017000*		0636587785000*		0686309017000*		0736000000000¤	
0786309017000¤		0836587785000¤		0886809017000¤		0936951057000¤	
0035923880000¤		0085707107000¤		0135382683000¤		0185000000000*	
0235382683000*		0285707107000*		0335923880000*		0385999999000*	
0435923880000*		0485707107000*		0535382683000*		0585000000000¤	
0635382683000¤		0685707107000¤		0735923880000¤		0785999999000¤	
0835923880000¤		0885707107000¤		0935382683000¤		0034891007000¤	
0084587785000¤		0134156434000¤		0184309017000*		0234707107000*	
0284951057000*		0334987688000*		0384809017000*		0434453990000*	
0484000000000¤		0534453990000¤		0584809017000¤		0634987688000¤	
0684951057000¤		0734707107000¤		0784309017000¤		0834156434000*	
0884587785000*		0934891007000*		0033852640000¤		0083453990000¤	
0133078459000*		0183587785000*		0233923880000*		0283987688000*	
0333760406000*		0383309017000*		0433233445000¤		0483707107000¤	
0533972370000¤		0583951057000¤		0633649448000¤		0683156434000¤	
0733382683000*		0783809017000*		0833996917000*		0883891007000*	
0933522499000*		0032809017000¤		0082309017000¤		0132309017000*	
0182809017000*		0232999999000*		0282809017000*		0332309017000*	
0382309017000¤		0432809017000¤		0482999999000¤		0532809017000¤	
0582309017000¤		0632309017000*		0682809017000*		0732999999000*	
0782809017000*		0832309017000*		0882309017000¤		0932809017000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0031760406000¤		0081156434000¤		0131522499000*		0181951057000*	
0231923880000*		0281453990000*		0331233445000¤		0381809017000¤	
0431996917000¤		0481707107000¤		0531078459000¤		0581587785000*	
0631972370000*		0681891007000*		0731382683000*		0781309017000¤	
0831852640000¤		0881987688000¤		0931649448000¤		0030707107000¤	
0080000000000*		0130707107000*		0180999999000*		0230707107000*	
0280000000000¤		0330707107000¤		0380999999000¤		0430707107000¤	
0480000000000*		0530707107000*		0580999999000*		0630707107000*	
0680000000000¤		0730707107000¤		0780999999000¤		0830707107000¤	
0880000000000*		0930707107000*		0029649448000¤		0079156434000*	
0129852640000*		0179951057000*		0229382683000*		0279453990000¤	
0329972370000¤		0379809017000¤		0429078459000¤		0479707107000*	
0529996917000*		0579587785000*		0629233445000¤		0679891007000¤	
0729923880000¤		0779309017000¤		0829522499000*		0879987688000*	
0929760406000*		0028587785000¤		0078309017000*		0128951057000*	
0178809017000*		0228000000000¤		0278809017000¤		0328951057000¤	
0378309017000¤		0428587785000*		0478999999000*		0528587785000*	
0578309017000¤		0628951057000¤		0678809017000¤		0728000000000*	
0778809017000*		0828951057000*		0878309017000*		0928587785000¤	
0027522499000¤		0077453990000*		0127996917000*		0177587785000*	
0227382683000¤		0277987688000¤		0327649448000¤		0377309017000*	
0427972370000*		0477707107000*		0527233445000¤		0577951057000¤	
0627760406000¤		0677156434000*		0727923880000*		0777809017000*	
0827078459000¤		0877891007000¤		0927852640000¤		0026453990000¤	
0076587785000*		0126987688000*		0176309017000*		0226707107000¤	
0276951057000¤		0326156434000¤		0376809017000*		0426891007000*	
0476000000000¤		0526891007000¤		0576809017000¤		0626156434000*	
0676951057000*		0726707107000*		0776309017000¤		0826987688000¤	
0876587785000¤		0926453990000*		0025382683000¤		0075707107000*	
0125923880000*		0175000000000¤		0225923880000¤		0275707107000¤	
0325382683000*		0375999999000*		0425382683000*		0475707107000¤	
0525923880000¤		0575000000000*		0625923880000*		0675707107000*	
0725382683000¤		0775999999000¤		0825382683000¤		0875707107000*	
0925923880000*		0024309017000¤		0074809017000*		0124809017000*	
0174309017000¤		0224999999000¤		0274309017000¤		0324809017000*	
0374809017000*		0424309017000¤		0474999999000¤		0524309017000¤	
0574809017000*		0624809017000*		0674309017000¤		0724999999000¤	
0774309017000¤		0824809017000*		0874809017000*		0924309017000¤	
0023233445000¤		0073891007000*		0123649448000*		0173587785000¤	
0223923880000¤		0273156434000*		0323996917000*		0373309017000*	
0423852640000¤		0473707107000¤		0523522499000*		0573951057000*	
0623078459000¤		0673987688000¤		0723382683000¤		0773809017000*	
0823760406000*		0873453990000¤		0923972370000¤		0022156434000¤	
0072951057000*		0122453990000*		0172809017000¤		0222707107000¤	
0272587785000*		0322891007000*		0372309017000¤		0422987688000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0472000000000*		0522987688000*		0572309017000*		0622891007000¤	
0672587785000¤		0722707107000*		0772809017000*		0822453990000¤	
0872951057000¤		0922156434000*		0021078459000¤		0071987688000*	
0121233445000*		0171951057000¤		0221382683000¤		0271891007000*	
0321522499000*		0371809017000¤		0421649448000¤		0471707107000*	
0521760406000*		0571587785000¤		0621852640000¤		0671453990000*	
0721923880000*		0771309017000¤		0821972370000¤		0871156434000*	
0921996917000*		0020000000000*		0070999999000*		0120000000000¤	
0170999999000¤		0220000000000*		0270999999000*		0320000000000¤	
0370999999000¤		0420000000000*		0470999999000*		0520000000000¤	
0570999999000¤		0620000000000*		0670999999000*		0720000000000¤	
0770999999000¤		0820000000000*		0870999999000*		0920000000000¤	
0019078459000*		0069987688000*		0119233445000¤		0169951057000¤	
0219382683000*		0269891007000*		0319522499000¤		0369809017000¤	
0419649448000*		0469707107000*		0519760406000¤		0569587785000¤	
0619852640000*		0669453990000*		0719923880000¤		0769309017000¤	
0819972370000*		0869156434000*		0919996917000¤		0018156434000*	
0068951057000*		0118453990000¤		0168809017000¤		0218707107000*	
0468000000000¤		0518987688000¤		0568309017000*		0618891007000*	
0268587785000*		0318891007000¤		0368309017000¤		0418987688000*	
0668587785000¤		0718707107000¤		0768809017000*		0818453990000*	
0868951057000¤		0918156434000¤		0017233445000*		0067891007000*	
0117649448000¤		0167587785000¤		0217923880000*		0267156434000*	
0317996917000¤		0367309017000*		0417852640000*		0467707107000¤	
0517522499000¤		0567951057000*		0617078459000*		0667987688000¤	
0717382683000*		0767809017000*		0817760406000¤		0867453990000¤	
0917972370000*		0016309017000*		0066809017000*		0116809017000¤	
0166309017000¤		0216999999000*		0266309017000¤		0316809017000¤	
0366809017000*		0416309017000*		0466999999000¤		0516309017000*	
0566809017000*		0616809017000¤		0666309017000¤		0716999999000*	
0766309017000¤		0816809017000¤		0866809017000*		0916309017000*	
0015382683000*		0065707107000*		0115923880000¤		0165000000000*	
0215923880000*		0265707107000¤		0315382683000¤		0365999999000*	
0415382683000¤		0465707107000¤		0515923880000*		0565000000000¤	
0615923880000¤		0665707107000*		0715382683000*		0765999999000¤	
0815382683000*		0865707107000*		0915923880000¤		0014453990000*	
0064587785000*		0114987688000¤		0164309017000*		0214707107000*	
0264951057000¤		0314156434000*		0364809017000*		0414891007000¤	
0464000000000*		0514891007000*		0564809017000¤		0614156434000¤	
0664951057000*		0714707107000¤		0764309017000¤		0814987688000*	
0864587785000¤		0914453990000¤		0013522499000*		0063453990000*	
0113996917000¤		0163587785000*		0213382683000*		0263987688000¤	
0313649448000*		0363309017000*		0413972370000¤		0463707107000*	
0513233445000*		0563951057000¤		0613760406000*		0663156434000*	
0713923880000¤		0763809017000*		0813078459000*		0863891007000¤	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0913852640000*		0012587785000*		0062309017000*		0112951057000□	
0162809017000*		0212000000000□		0262809017000□		0312951057000*	
0362309017000□		0412587785000□		0462999999000*		0512587785000□	
0562309017000□		0612951057000*		0662809017000□		0712000000000*	
0762809017000*		0812951057000□		0862309017000*		0912587785000*	
0011649448000*		0061156434000*		0111852640000□		0161951057000*	
0211382683000□		0261453990000□		0311972370000*		0361809017000□	
0411078459000*		0461707107000*		0511996917000□		0561587785000*	
0611233445000*		0661891007000□		0711923880000*		0761309017000□	
0811522499000□		0861987688000*		0911760406000□		0010707107000*	
0060000000000□		0110707107000□		0160999999000*		0210707107000□	
0260000000000*		0310707107000*		0360999999000□		0410707107000*	
0460000000000□		0510707107000□		0560999999000*		0610707107000□	
0660000000000*		0710707107000*		0760999999000□		0810707107000*	
0860000000000□		0910707107000□		0009760406000*		0059156434000□	
0109522499000□		0159951057000*		0209923880000□		0259453990000*	
0309233445000*		0359809017000□		0409996917000*		0459707107000□	
0509078459000*		0559587785000*		0609972370000□		0659891007000*	
0709382683000□		0759309017000□		0809852640000*		0859987688000□	
0909649448000*		0008809017000*		0058309017000□		0108309017000□	
0158809017000*		0208999999000□		0258809017000*		0308309017000□	
0358309017000□		0408809017000*		0458999999000□		0508809017000*	
0558309017000□		0608309017000□		0658809017000*		0708999999000□	
0758809017000*		0808309017000□		0858309017000□		0908809017000*	
0007852640000*		0057453990000□		0107078459000□		0157587785000*	
0207923880000□		0257987688000*		0307760406000□		0357309017000*	
0407233445000*		0457707107000□		0507972370000*		0557951057000□	
0607649448000*		0657156434000□		0707382683000□		0757809017000*	
0807996917000□		0857891007000*		0907522499000□		0006891007000*	
0056587785000□		0106156434000*		0156309017000*		0206707107000□	
0256951057000*		0306987688000□		0356809017000*		0406453990000□	
0456000000000*		0506453990000*		0556809017000□		0606987688000*	
0656951057000□		0706707107000*		0756309017000□		0806156434000□	
0856587785000*		0906891007000□		0005923880000*		0055707107000□	
0105382683000*		0155000000000□		0205382683000□		0255707107000*	
0305923880000□		0355999999000*		0405923880000□		0455707107000*	
0505382683000□		0555000000000*		0605382683000*		0655707107000□	
0705923880000*		0755999999000□		0805923880000*		0855707107000□	
0905382683000*		0004951057000*		0054809017000□		0104587785000*	
0154309017000□		0204000000000*		0254309017000*		0304587785000□	
0354809017000*		0404951057000□		0454999999000*		0504951057000□	
0554809017000*		0604587785000□		0654309017000*		0704000000000□	
0754309017000□		0804587785000*		0854809017000□		0904951057000*	
0003972370000*		0053891007000□		0103760406000*		0153587785000□	
0203382683000□		0253156434000□		0303078459000□		0353309017000*	

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0403522499000□		0453707107000*		0503852640000□		0553951057000*	
0603996917000□		0653987688000*		0703923880000□		0753809017000*	
0803649448000□		0853453990000*		0903233445000□		0002987688000*	
0052951057000□		0102891007000*		0152809017000□		0202707107000*	
0252587785000□		0302453990000*		0352309017000□		0402156434000*	
0452000000000□		0502156434000□		0552309017000*		0602453990000□	
0652587785000*		0702707107000□		0752809017000*		0802891007000□	
0852951057000*		0902987688000□		0001996917000*		0051987688000□	
0101972370000*		0151951057000□		0201923880000*		0251891007000□	
0301852640000*		0351809017000□		0401760406000*		0451707107000□	
0501649448000*		0551587785000□		0601522499000*		0651453990000□	
0701382683000*		0751309017000□		0801233445000*		0851156434000□	
0901078459000*		0751309017000□		0801233445000*		0851156434000□	

IX. APPENDIX C: L.S.II M PROGRAM

A.Form of the L.S.II M Program

1. Modifications made to L.S.II

The modified least squares program (L.S.II M) provides convenient facilities for programming structure factor evaluations involving multiple term structure factors. The Senko and Templeton L.S.II (12) program was designed to handle only single (orthorhombic) term structure factors.

There are four important changes made to the L.S.II program to produce the L.S.II M. A new loading routine is used so that more space is available on the drum for programming. The scale factor storage locations are expanded to allow for a total of 10 scale factors by moving the orders in 0678 and 0679. A small subroutine is inserted just before the make up of arguments section. This subroutine will zero all of the work cells used as temporary storage for the trigonometric term routines. The storage orders for these temporary work cells have been changed to add and store pairs which accumulate results of successive passes through the trigonometric term routines. The orthorhombic terms may be summed in the desired sequence by modifying the term routine exits. This is sufficient for triclinic and monoclinic space groups. For space groups of greater symmetry, a modification of the indices may be made and a new set of

terms can be added to the previous results. This may be repeated until the structure factor is obtained. The derivatives of the structure factor are obtained automatically when this procedure is used.

2. Programming information

The trigonometric part of the structure factor should be expressed in the form

$$\sum_{i=1}^{n} \sum_{j=1}^{m} T_{ij}(2\pi\, t_{il}x)\; T'_{ij}(2\pi\, t'_{il}y)\; T''_{ij}(2\pi\, t''_{il}y)$$

where the T_{ij} are either sine or cosine functions, and the t_{il} are functions of h, k, ℓ. The product of $T_{ij}\; T'_{ij}\; T''_{ij}$ must be one of the available orthorhombic terms. The summation over j is carried out by linking orthorhombic type subroutines and the summation over i is carried out by modifying the t's and repeating the summation over j.

If n = 1, no argument modification is required and a simple modification of the term exits is all that is required. The eight term routines are divided into two types, depending on whether the term is stored as the A or B part of the structure factor. The terms and related information are given in Table 22. For example, if the desired structure factor is cos 2πhx cos 2πky cos 2πℓz - sin 2πhx sin 2πky sin 2πℓz, the "A code" on the detail card may be 1408. The exit of the 1408 routine at 1462 is modified to give 21 1704 1558 so that the

Table 22. Orthorhombic structure factor terms

T_{ij}	T'_{ij}	T''_{ij}	Code type	Address	Normal exit	Normal exit order
sine	cosine	cosine	B	1528	1483	21 1729 0796
cosine	sine	cosine	B	1428	1545	21 1729 0796
cosine	cosine	sine	B	1478	1563	21 1729 0796
-sine	sine	sine	B	1578	1971	21 1729 0796
cosine	cosine	cosine	A	1408	1462	21 1704 1999
-cosine	sine	sine	A	1458	1976	21 1704 1999
-sine	cosine	sine	A	1508	1985	21 1704 1999
-sine	sine	cosine	A	1558	1994	21 1704 1999

1558 routine is forced to follow. It should be noted that A code type terms cannot be coupled with B code type terms in this way as different work cells are used.

If a summation over i is required, the procedure is a little more complicated. The summation over j for each i is accomplished in the same manner as above. More than one such pass through the term routines is required in order to sum over i. Each pass must be followed by an argument (t) modification routine which either prepares the new arguments or restores the original conditions and exits to the

remainder of the program at 1610. If a new pass through the term routines is required the argument modification routine must exit to 1433 which is the make up of arguments routine. The argument modification routine must be written anew for each new form of the structure factor summation. The first order of the argument modification routine is usually at 1999. The last desired term exit must refer to the start of the appropriate make up of arguments address. The first pass through the term routines is made with the normal indices stored in the following fashion:

0303 has h (t)
0353 has k (t') with decimal point at 0,
0403 has ℓ (t")

1459 and 1484 have h (t)
1509 and 1534 have k (t') with decimal point at 2.
1559 and 1584 have ℓ (t")

The argument modification routine operates on these cells to form the new t, t' and t". After the last pass through the term routines these cells and the argument modification routine must be restored to their original condition. There is a short section of the original program which may be used in the argument modification routine. This section will generate the contents of 1459, 1484, 1509, 1534, 1559 and 1584 from the contents of 0303, 0353 and 0403. This routine

is entered at 1409 with ℓ (t") in 8003 after locations 0303, 0353 and 0403 have been modified. The normal exit is at 1451 with 24 1459 1894. Since this routine is not needed while the sum over i is carried out, the exit may be modified to 24 1459 XXXX, where XXXX refers to the appropriate argument modification address, when the argument modification routine is first entered. This must be reset before final exit to 1610. Locations 1901 to 1926 and 1937 to 1942 can be used for the modification routine. There are other spaces including part of the atomic band which are available if required. Unless modification is made the program computes the normal orthorhombic structure factor.

The modification cards are loaded with the normal modification cards before the "to S.F." card. The form is
00 000X YYYY word 1 word 2 ... word 7, where X is the number of words to be loaded from the card and YYYY is the address of word 1. The other words are stored sequentially. An exception is 1999, which is loaded with
00 0000 1952 69 1953 1954 word 1 24 1999 1996 .

B. Operating Instructions

1. Assembly of input deck

The deck is loaded in the following sequence:

LS-IIM2 deck,

modification cards,

limit card,
scale factor cards,
standard deviations card,
weighting factor card,
parameter cards,
temperature factor cards,
TO SF card,
CYCLE ZERO cards (5 cards),
a set of detail cards for each layer in the order

KTn card,
reflection cards for nth layer,
NK card.

The last NK card is replaced by an LK card.

2. Console operation

a. Switch settings The console switches are set as follows:

storage entry 70 0001 0003,
programmed not significant,
half cycle run,
address selection not significant,
control run,
display program register,
overflow stop,
error stop.

b. Start program To start the program depress computer reset, program start and start the read feed and the punch feed.

3. Subsequent cycles

With all parameters varying reload input deck beginning with item 10 and start the read feed and the punch feed; do not touch console.

With some parameters held constant or with modification changes place TO LR card in front of the scale factor cards, parameter cards, or temperature cards containing the

parameters to be held constant, modification cards and the input deck beginning with item 9. Place this deck in the read feed. Start the read feed and the punch feed but do not touch console.

4. Description of input cards

The NK cards have the form

00 0000 0000 61 0832 0692 12 3456 7890 61 0882 0601
00 0000 1394 01 2345 6789 01 2345 6789 00 0000 0000 .

The LK card has the form

00 0000 0000 61 0832 0692 71 1910 1216 61 0882 0601
69 1107 1956 24 1954 1957 60 0432 1191 00 0000 0000 .

The KT"n" card has the form

00 0000 0000 60 1633 1953 19 067X 1954 35 0002 1955
21 1632 1394 00 0000 0000 00 0000 0000 00 0000 0000 .

The set sums to zero (5 cards) are loaded in the following order:

00 0000 0000 24 0332 1953 24 0382 1954 24 0432 1955
24 0482 1956 24 0532 1957 24 0582 1958 24 0632 1394 ,
00 0000 0000 24 0682 1953 24 0932 1954 24 0832 1955
24 1768 1956 24 1793 1957 24 1769 1958 24 1794 1394 ,
00 0000 0000 24 1770 1953 24 1795 1954 24 1771 1955
24 1796 1956 24 1772 0649 69 1958 0642 21 1876 1715 ,
00 0000 0000 69 1951 1953 24 1728 1954 24 1729 1955
24 1726 1956 24 1727 1394 00 0000 0000 00 0000 0000 ,

00 0000 0000 69 1953 1954 19 0632 1105 24 1109 1955
69 1956 1957 35 0002 1116 24 1105 1394 00 0000 0000 .

The TO S.F. card has the form

00 0000 1394 ... .

The TO L.R. card has the form

00 0000 0000 00 0000 1996 ... .

The do not punch structure factors card has the form

00 0001 0574 00 0000 1895 ... .

The punch structure factor card has the form

00 0001 0574 71 1927 1895 ... .

The constant weighting factor cards are

00 0001 0354 60 1928 1683 ... ,

00 0001 1378 00 0000 8000 ... .

The above cards do not vary from one calculation to another and may be punched up once and filed with the program deck. The cards described below contain the required information for each structure.

The limit card is 00 0001 1860 20 XXXX 0000 ... , where XXXX = 0250 + 50 n, ($n \leq 16$). n is the number of independent atoms.

The scale factor cards have the form

00 0001 067Y $K_y(8)$ ... , where Y is the layer number ($0 \leq Y \leq 9$).

The standard deviations card is 00 0001 0900 $4\pi^2(u-v)$ (4) ... , where u is the number of independent F values and v is the number of parameters being varied.

The parameter cards have the form

00 0003 bbbb X_n (10) Y_n (10) Z_n (10) ... , where bbbb = 0255 + 50 n, (1 n 16).

The temperature factor cards have the form

00 0002 cccc B_n/λ^2 (5) 19 195X dddd ... , where cccc = 0280 + 50 n, X is the field containing the scattering factors for atom n, dddd is the code controlling the multiplication of the scattering factor by a constant. These factors are listed in Table 23. Other factors may be substituted for these by loading them into the appropriate locations.

Table 23. Multiplicative factors

dddd	Factor	Location
0442	1	-
0317	1/2	0325 (10)
0318	1/4	0326 (10)
0319	1/8	0327 (10)

The reflection cards (detail cards) have the form

hh kk $\ell\ell$ abcd I (7):F (2) $\sin^2\theta$ (10):e f_1 (6):A f_2 (6) f_3 (6) f_4 (6):B f_5 (6) . a, b, and c give the signs of h, k, and ℓ with 8 for plus and 9 for minus. d is 8 for an

observed reflection and 9 for unobserved reflections. e is 8 if $F_o \geq 4F_{min}$ and is 9 otherwise. A and B are the structure factor term routine codes as shown in Table 22. The f_i are scattering factors.

5. Description of output cards

Where applicable, all output cards are of the correct format for use as input cards for subsequent cycles if it is necessary to reload the program.

a. Layer output Structure factor cards have the form

$$0h0k0\ell \begin{matrix}8888\\9999\end{matrix} K_y F_o(5) : \sin^2\theta(4)\ F_c(5)\ F_o\text{-}F_c(5)\ A_o(5)$$

$$A_o\text{-}A_c(5)\ B_c(5)\ B_o\text{-}B_c(5)\ .$$

Scale factor cards have the form

$$00\ 0001\ 067y\ K_y(8)\ \epsilon K_y(8)\ R_3 \text{ for layer } (10)\ .$$

b. Finish output The reliability factor card is

$$R_1(10)\ R_2(10)\ R_3 \text{ all data}(10)\ R_3 \text{ last layer } (10)\ .$$

Atomic cards in sets of three are then punched in the following order:

Temperature factor card

$$00\ 0002\ cccc\ \frac{B_n}{\lambda^2}(5)\ 19\ 195x\ dddd\ \frac{\epsilon B_n}{\lambda^2}(5)\ ,$$

Parameter card

$$00\ 0003\ bbbb\ x_n(10)\ y_n(10)\ z_n(10)\ \epsilon x_n(10)$$

$$\epsilon y_n(10)\ \epsilon z_n(10)\ , \text{ and the}$$

Atomic standard deviations card

$$0 \quad 0 \quad 0 \quad 0 \quad \sigma x_n \quad \sigma y_n \quad \sigma z_n \ .$$

R_1, R_2 and R_3 are defined by

$$R_1 = \frac{\Sigma |F_o| - |F_c|}{\Sigma |F_o|} \ , \quad R_2 = \frac{\Sigma (|F_o| - |F_c|)^2}{\Sigma |F_o|^2} \ , \text{ and}$$

$$R_3 = \frac{\Sigma w(|F_o| - |F_c|)^2}{\Sigma \ w|F_o|^2} \ .$$

6. Plug board

The plug board for the I.B.M. 650 is the same as that used for the L.S.II program which is 8 words straight in and 8 words straight out. A Y-punch in column 1 is used to identify load cards.

7. Program deck

The program cards are listed in Table 24, and must be kept in the order shown. Each line contains the contents of one card.

TABLE 24. PROGRAM CARD LISTING FOR L.S. 2 M (EACH ROW CONTAINS THE CONTENTS OF ONE CARD WITH SYMBOLS * AND ¤ REPRESENTING X/0 AND Y/0)

```
COL.     10        20        30        40        50        60        70        80

000001000¤16000180B690005000D240000000F70185118 5A65000780B21199000B000000000¤
G01801180A691852185A691854185C691856185E691858185G701895189E691856185H241899189I
F91852180B241895180C691853180D241896180E691854180F241897180G691855180H241898185G
B41996189F701997199G241997189G601951196B241962189H300004197C241973189I441978800A
B41978189F300002199¤241990189G691981196E241981189H240000196A241965189I221981197¤
B41970189F300004198F241986189G151992195¤241992189H691952800B241950189I221987196F
B41966189F601992196H241968189G151981800C241961189H101964196I241964189I000001000¤
B41969189F158001197G241977189G201981198D241984189H111987199A241991189I441995199F
B41995199F108001800C000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007000¤000009990¤009009990¤016009990¤022009990¤028009990¤034009990¤041009990¤
000007000G047009990¤053009980¤060009980¤066009980¤072009970¤078009970¤085009960¤
000007001D091009960¤097009950¤103009940¤110009940¤116009930¤122009920¤128009910¤
000007002A135009910¤141009900¤147009890¤153009880¤159009870¤166009860¤172009850¤
000007002H178009840¤184009820¤190009810¤197009800¤203009790¤209009780¤215009760¤
000007003E221009750¤227009740¤233009720¤240009710¤246009690¤252009680¤258009660¤
000007004B264009640¤270009630¤276009610¤282009590¤288009580¤294009560¤300009540¤
000007004I306009520¤312009500¤318009480¤324009460¤330009440¤336009420¤342009400¤
000007005F348009380¤353009350¤359009330¤365009310¤371009280¤377009260¤383009240¤
000007006C388009210¤394009190¤400009160¤406009140¤411009110¤417009090¤423009060¤
000007007¤429009030¤434009000¤440008980¤445008950¤451008920¤457008890¤462008860¤
000007007G468008830¤473008800¤479008770¤484008740¤490008710¤495008680¤501008650¤
000007008D506008620¤511008590¤517008560¤522008520¤528008490¤533008460¤538008420¤
000007009A543008390¤549008360¤554008320¤559008290¤564008250¤569008220¤575008180¤
000007009H580008140¤585008110¤590008070¤595008030¤600008000¤605007960¤610007920¤
000007010E615007880¤620007840¤625007800¤630007770¤635007730¤639007690¤644007640¤
000007011B649007600¤654007560¤659007520¤663007480¤668007440¤673007400¤677007350¤
000007011I682007310¤687007270¤691007220¤696007180¤700007140¤705007090¤709007050¤
000007012F714007000¤718006960¤722006910¤727006870¤731006820¤735006770¤740006730¤
000007013C744006680¤748006630¤752006590¤756006540¤760006490¤764006440¤769006390¤
000007014¤773006350¤777006300¤780006250¤784006200¤788006150¤792006100¤796006050¤
000007014G800006000¤803005950¤807005900¤811005850¤814005800¤818005750¤822005690¤
```

TABLE 24. CONTINUED

```
COL.     10          20          30          40          50          60          70          80

000007015D825005640¤829005590¤832005540¤836005490¤839005430¤842005380¤846005330¤
000007016A849005280¤852005220¤856005170¤859005110¤862005060¤865005010¤868004950¤
000007016H871004900¤874004840¤877004790¤880004730¤883004680¤886004620¤889004570¤
000007017E892004510¤895004450¤898004400¤900004340¤903004290¤906004230¤909004170¤
000007018B911004110¤914004060¤916004000¤919003940¤921003880¤924003830¤926003770¤
000007018I928003710¤931003650¤933003590¤935003530¤938003480¤940003420¤942003360¤
000007019F944003300¤946003240¤948003180¤950003120¤952003060¤954003000¤956002940¤
000007020C958002880¤959002820¤961002760¤963002700¤964002640¤966002580¤968002520¤
000007021¤969002460¤971002400¤972002330¤974002270¤975002210¤976002150¤978002090¤
000007021G979002030¤980001970¤981001900¤982001840¤984001780¤985001720¤986001660¤
000007022D987001590¤988001530¤989001470¤990001410¤991001350¤991001280¤992001220¤
000007023A993001160¤994001100¤994001030¤995000970¤996000910¤996000850¤997000780¤
000007023H997000720¤998000660¤998000600¤998000530¤999000470¤999000410¤999000340¤
000007024E999000280¤999000220¤999000160¤999000090¤999000030¤999000000¤951610000¤
000007025B861109048D779108187C70507408B63790670 3B577206065C522305488A472504965H
000007025I427604493C386904065G350103678H316803328G286603011I259302725C234702466¤
000007026F212302231C192202019¤173801826H157301653¤142301495G128801353D116601224F
000007027C105401108¤095401002F086400907B078100820H070600742G064000672A057900608A
000007028¤052300550B047400497I042900450E038800407F035100368H031700333G028800302¤
000007028G026000273B023500247B021300223G019200202D017500183B015700165G014300150¤
000007029D012900135G011700122H010600111A009500100E008700091¤007800082C007100074E
000004030A006400067D100332035B000000000C601559156F008700091¤007800082C007100074E
000007031G608003032B608003032C608003032D201927163A000000195B190325044B190326044B
000006032D190327044B500000000¤250000000¤125000000¤668002163H191582141C190326044B
000007034A191654142A210303135G072000000*241550144E241550152¤241550140C241550145C
000007034H210353136¤600523042G600403150G658002176¤210332035D000000000K691953081H
000007036G608003037B608003037C608003037D350002147G608003178G190425044B190426044B
000006037D190427044B062500000¤031250000¤015625000¤668002163G191582148H190426044B
000007039A191604147A210517052¤460396039G211770175B211603160G691699185C691650185C
000007039H211771039I601603164H000017676D108001042E691927074H000000000D600517047E
000007041G101770039D101771039H101772179H191380154F101726039B191767161G241576142¤
000006042D211928030B210382034I191632042D198001138C690382044D191532141C241576142¤
```

TABLE 24. CONTINUED

```
COL.     10        20        30        40        50        60        70        80

000007044A191654152A210447140¤000000000¤350002040A040000000¤210400040D000091588¤
000007044H241851171¤678003061I200432049I108001047F000012256E350004037A101928040B
000007046G690420042C191379144F191380149F191379159F241576142¤241576149E241576149E
000006047D690477139B198001138A210482049H300002057B690482049C191532148H241576149E
000007049A191604157A100445800C350002045A618002045D000099246E200452061G150400047D
000007049H600523169D601930138E191930138G210632059E110517052I601612057¤211612051I
000007051G000000000¤698003052D198001057I600523139C123456789¤191928071G000000000¤
000006052D231378138D191378057E198001057G211932054H211933050B211934055B000000000¤
000007054A600495135B190495059I601378054D191928059G608002050D210532050C110523052G
000007054H600452052B210582054C240523055A211772171E601378050¤240517062¤608002056I
000007056G350005042F691928138F210573052F190573057H100682059C160625067I000698280¤
000006057D711927189E201680054A241936057D100532054F100632050A100582054I000698280¤
000007059A690551059B241798171E210682059A690443055C651953056H231928073B300002055D
000007059H641929049F201755179G000001067A100582060B240882060C640782069F000001000¤
000007061G608002052E190573057A150432045¤240523057F651957071I690825067H601928074A
000006062D000000000¤000001000¤000000000¤000000000¤230795800A690641064D601928074A
000007064A211772162E241861064E600749090D241798139D690646064G461868064H241865171E
000007064H690650065A240882195G211876187I241861065B690653070A461868182¤350004086G
000007066G350004137G690718072A100000000¤036479845H012575551I023741905C007394878¤
000006067D006718064B000000000¤000000000¤000000000¤241378069I460891074B007394878¤
000007069A240694195C100532069C240832069E000000000¤210782074C201930069G711910195E
000007069H711910120C601928168C190340084C241865182¤690718077A310004077E210870087C
000007071G350004052H000001163C698003062H210000000¤230600077D201928070B610682079C
000006072D211928074E210770082C000000000¤210749119¤190746077B151633082B610682079C
000002073B201888059D000000000¤000000000¤210749119¤190746077B151633082B610682079C
000007074A110794084I158001085¤660932079B608002075C650749085D700000000*350002080D
000007074H910802085C210670072D350004076G300004076H200447140¤191632075A240932075¤
000007076G640782074D608002072H608002077I000000005C241927089B211929079I241927118¤
000006077D241927064C608002128F000000000¤000000000¤690443079G191633070C241927118¤
000007079A190340074G150632075D198001080C000010000¤000000000¤651954071I241851087A
000007079H310008091G101632074I000000000¤000000000¤211930044I350002081G210720072C
000007081G100720072E910622062C201930049H77777777G201378069I201633072B440829084A
```

TABLE 24. CONTINUED

```
COL.     10          20          30          40          50          60          70          80

000006082D641928082A000000040¤000000000¤000000000¤000000000¤600632070¤440829084A
000007084A690820077C190312065D35004070D000000000¤000000000¤000000000¤000000000¤
000007084H000000000¤460622085B20192904 9D000000000¤650669082D460868081I300004066H
000007086G100870079H611929080B000000000¤000000000¤241876173C000000000¤610682084B
000006087D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤6106820848
000007089A241929049D711910110¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007089H000000000¤000000000¤400000000¤000000000¤000000000¤000000000¤100604072G
000007091G640770076I000000000¤000000000¤000000600¤000000000¤000000000¤000000000¤
000006092D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007094A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007094H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007096G000000000¤000000000¤000000000¤000000900¤000000000¤000000000¤000000000¤
000006097D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001098B000000200¤690305180H690308181A111852800C21936194¤601897800C601898800C
000007099A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007099H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007101G000000000¤000000000¤000000000¤000000020¤000000000¤000000000¤000000000¤
000006102D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007104A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007104H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007106G000000000¤000000000¤000000000¤000010000¤000000000¤000000000¤000000000¤
000006107D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007109A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007109H000000000¤000000000¤600532113G101158114F101158114H000000000¤3500021116
000007110E350001111F241934114¤711910120C241928113D190312110E000000000¤2419291188
000007111B190920111C210870120E210870118C100870116E100870112E210870112C691171112F
000007111I310004113¤000017000¤310001112I241020112G610682110I201929120A310001113F
000007112F231171117D198001116G201931120H640982112D691283128G241070113C191070114G
000007113C191020115B600920113B000000000¤640770112I190312110D000000000¤2108701206
000007114¤711910132I000000000¤441146110A711910195D441148110B640382117B210920120D
000007114G350003111D210970111B651202115G241934118I350000131C350003111E000000000¤
000007115D000000000¤601158125¤000000000¤310004111H100000000¤000000000¤000000000¤
```

TABLE 24. CONTINUED

```
COL.     10          20          30          40          50          60          70          80

000007116A201927116B600482114E640770127¤100870116C640770127A241120117F100870117E
000007116H241930121B600970120F000000900¤000001043¤201928118A241931121B241927119¤
000007117E441221122B350003113I191120119D201933121¤000000000¤210770124B600582118G
000007118B651208111I611020117G690820117C201928120B690443110F640532118H201929195C
000007118I241936195D690443119F640332116A000000000¤350000131F350003116D441250115E
000007119F241930119G241931119H241932119I241933115¤000000000¤150330118E200330114I
000007120C600337114B600339114D610316112B190313116F610315113A150305120I200305110H
000007121¤150307121A200307116H600338119E600314127F150306121E200306111A600312121G
000007121G640340112A000000000¤000000000¤310001127G360000118¤451223118D300001122D
000007122D200770122E651226122G000009000¤691176122H221176122I691152123¤221152123A
000007123A691147123B221147123C691194123D221194123E691193123F221193123G691151124¤
000007123H601241129F201929072I221151116I150330118E350008124C658002124D300004122G
000007124E000000000¤000000000¤000000000¤000000000¤000000000¤211170121C000050000¤
000007125B000000000¤000000000¤241275129D461258125I211275125I000000000¤691261126D
000007125I601293800C000000000¤461288129¤000000000¤000000000¤241285123H111268127C
000007126F000000000¤000000000¤050000000¤658003123I300001117H300001112H151275127I
000007127C111201125E111278128E000050000¤641170122¤201932121D201217000¤101282800C
000007128¤691284129B241285128¤050000000B000003040E210670072D461288121F190746126I
000007128G231283128I101291129E241927118F691251125D151217999H240749139D151201127B
000007129D691299128A608003800C111201125F000000000¤601860126E461288121F300003130I
000007130A000000000¤000000000¤000000000¤300003115A191314130D000000000¤300003119C
000007130H000000000¤201314131G651314134G000000000¤640970132H640770132H000017500¤
000007131E640920133F640770133F600970132E000000000¤350007134B241928132A241929132B
000007132B241930132D241933134¤241934132F451330133E711910129H451305131¤691332139B
000007132I600582133G191314130G000000000¤698002132C691338139B651314131I651314134H
000007133F691339139B640900130¤698002134D698002134E690443134F600920132G641170133C
000007134C000000000¤241932134A241931133D241927132¤350007131B350007131E000000000¤
000007135¤300002057B000000005¤191928066G201359138H191359139G300001136A101359136C
000007135G678002137C210523177F000017945I678002137B168002136I168001137¤168002137A
000007136D668002032¤690468047A690469047B690470047C241575035¤198001135F461382139¤
000007137A648001136B961637037H951638032H000000000¤300004059H641929164¤211931054G
000007137H000000800¤997000720¤072000000*300006049G158001138I350004044F608001054B
```

TABLE 24. CONTINUED

```
COL.     10          20          30          40          50          60          70          80

000007138E198001047H300006059F300002054E651391139E158001139H158001135¤500000000¤
000007139B451396800A101701135H701951173C108001135D241350135C658003135F101351135E
000007139I601378054B600303140G000000000¤000000000¤191561143H611459141D611509141E
000007140F611559141F191761143E601561136E608003037¤350002147E000000000¤000000000¤
000007141C608002142¤691417164F691418034F691419034G191654144G191654144H1916041441
000007142¤191575157¤211726152I211727148¤211728148A211729079F000000000¤000000000¤
000007142G000000000¤601582143G611484159A611534148I611584144A000000000¤000000000¤
000007143D691663152E691538169B000000000¤690341034D608002144E691442167A691443162A
000007144A691444162B191380147C191379152B191380152D191500159E211701140D211702140E
000007144H211703140F211704161¤600353145G241459189D191663155B191561146C601459146D
000007145E611509146E611559146F191762148E611561136F000000030¤000000000¤000000000¤
000007146B000000000¤608002152¤691467164G691468034G691469034F191604149G191380149H
000007146I191654149I000000000¤211726142I211727153¤211728153A211729079F211534150A
000007147F211484145A211584155A601582148G601484144¤601534149A611584154A000000000¤
000007148C000000000¤000000030¤691639169B000000000¤690391034E608002149E691492182B
000007149¤691493162A691494162A191379152C191379147D191379142C191500157¤211701145D
000007149G211702145E211703145F211704161¤760000000*241509153C211511152G191511146C
000007150D611459151D601509151E611559151F191763153E611511046G000000020*000000000¤
000007151A000031323¤000000000¤000000000¤691517034G691518164G691519164F191604154G
000007151H191604154H191654154I191575159E211726147I211727143¤211728143A211729079F
000007152E241379158E241380143D241532153F601532153G611484153I611534143I601584149¤
000007153B000031323¤600303156¤000000020*691588169B600447145B690441034E190447150B
000007153I691542182B691543162B691544167A191379142B191380157C191380142D000000000¤
000007154F211701150D211702150E211703150F211704161¤191604159I241559158C211561157G
000007155C191511143H611459156D611509156E000000000¤000000000¤611511136G000000040¤
000007156¤350002147F000086093¤000000000¤000000000¤691567034F691568164F691569164G
000007156G191654159G191654159H191604159I608003157F211726157I211727158¤211728158A
000007157D211729079F649007600*191379159F241582145¤611532158G611484158I611534154¤
000007158A611584159¤000086093¤600353141¤000000040¤241654062A000000000¤690491034D
000007158H241604152F691592167A691593182B691594162B191380157B191379157D191380147B
000007159E608003155¤211701155D211702155E211703030D211704161¤601803170I601755166¤
000007160B601755166A000424124C072000000*691663136H198001169A198001164A9403201360
```

TABLE 24. CONTINUED

```
COL.     10        20        30        40        50        60        70        80

000007160I191612041H600517042A101769165F000276059Q198001164B101768175G211672167E
000007161F211624162G211674167G101672162H101623167H101624173B241576032I241576042I
000007162C004467259F000925298*601803061H601680168F601680168G618003163E111883184F
000007163¤101883184E350002034B002300000¤010000000¤000000010¤191888164C450019006I
000007163G350002164E350002034H241500160E200495139I101795175D101796185H3000011641
000007164D211653160F210403140I241550150C241550155C191753041I201803170F650000170H
000007165A191804178B601755166B000917045P997000720¤211794174H211769165B211793174G
000007165H191612161A191612041G191764161E191765166E191766161F997000720¤191767161G
000007166E211623162F350005167I000025002E350005168A461722167C101674168B241576037I
000007167B000005417F161676173A000156499C601680168E000500000¤601680168H608003169E
000007167I608002174¤028189950¤618002174¤608003039E198001042H240442180F191789161H
000007168F191790161I191791162¤191792167¤000250000¤101793165G101794165E241746035A
000007169C461696169G300004137F211753170G691749185C691700185C601603160I660000175I
000007170¤660000170H000023734¤019570330E004053578000068559 7H451608032A608002161C
000007170G198001169¤201663166H191612161D241876062I101667177C101667172C101667172D
000007171D101667187D651768182C651769182D651770182E651771182F651772182G651793180¤
000007172A608003165A151676173A691727800C691728800C108001183B000001713R0014133020
000007172H000292735F009493632B300006174E461734173E608003164D651951170E151689169C
000007173E161689039C111744179I111744175¤111744175A110445185D210343174F651794180A
000007174B651795180B651796185I000024002D108001045C241604152F601753165H601653165I
000007174I650000175I691703800C691704800C601755042B004427418F211795169H228266950¤
000007175F650238170H211768160B000049416D201663166F300003166I352000000¤181333333D
000007176C253000000*000023734¤019570330E004053578000068559 7H000000000¤000000000¤
000007177¤000000000¤000000000¤000000000¤691726800C190000173¤211880178C601880184D
000007177G111884184F111885184F111886184F111887184F101785189B691835188I601786184H
000007178D350006184I000050000¤000049714M191955031G000000000¤000001713R0014133020
000007179A000292735F009493632B000000000¤000000000¤000000000¤000000000¤600517137E
000007179H211772162E691702800C101855187C101856187C101857187C001143639000000014¤
000007180E101758186C658003186D161860186E241761186I241762186I241763186F241764186I
000007181B241765186I241766186I241767187E241768187E241769187E241770187E241771187E
000007181I241772160A690443044H461725188B241576047I461629163¤461777182H461778182I
000007182F461779183¤461780183A101884184E101885184E101886184E101887184E101636049B
```

TABLE 24. CONTINUED

```
COL.     10        20        30        40        50        60        70        80

000007183C241786189C241787189C210447140¤241789189C241790189C241791189I2417921891
000007184¤241793189I241794189I241795189I241796189I691701800C101851800C111851800C
000007184G608003180E191953189A618002188A678003180G000000000¤000024002D221756800A
000007185D111860182A200337174A200338174B200339174C211796160¤101862187C200650000¤
000007186A211876187I200340185¤691721168D151867187A461868182¤111870177E000251000¤
000007186H601876178A101872800C449999009I691774187G000025002E101876800C691729800C
000007187E101878800C000000000¤221881178D000025002E101898800C240408171A190289173¤
000007188B601952056G200312171F200313171G200314171H200315171I200316172¤000000213¤
000007188I240442075B240442184H461847180F211851186A111896800C601897800C601898800C
000005189F000024002D690305180H690308181A111852800C211936194¤601897800C601898800C
000001111H691998112F000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001112D201930120A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001117D241927194E000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000003140¤600000140A201701140B201726141A000000000¤000000000¤000000000¤000000000¤
000002141A201702141B201727142E000000000¤000000000¤000000000¤000000000¤000000000¤
000004142A101726151¤101727151B101728151C101729154E000000000¤000000000¤000000000¤
000003142E201703142F201728142G201704143B000000000¤000000000¤000000000¤000000000¤
000002143B201729143C600303140G000000000¤000000000¤000000000¤000000000¤000000000¤
000001143F211701140D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001143F211701140D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000004144F101701143F101702146¤101703146A101704146B000000000¤000000000¤000000000¤
000003144G101702146¤101703146A101704146B000000000¤000000000¤000000000¤000000000¤
000003146¤211702140E211703140F211704199I000000000¤000000000¤000000000¤000000000¤
000001147¤211727143¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000004147A101726155F101727155G101728156B101729156C000000000¤000000000¤000000000¤
000002148B211728143A211729079F000000000¤000000000¤000000000¤000000000¤000000000¤
000001148F211726147I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000004149F101701197B101702197D101703197E101704197F000000000¤000000000¤000000000¤
000001151¤211726152I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000002151B211727148¤211728148A000000000¤000000000¤000000000¤000000000¤000000000¤
000004152A101726148F101727147¤101728148B101729148C000000000¤000000000¤000000000¤
000001154E211729079F000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
```

TABLE 24. CONTINUED

```
COL.     10         20         30         40         50         60         70         80

000004154F101701197I101702198¤101703198B101704198E000000000¤000000000¤000000000¤
000002155F211726142I211727153¤000000000¤000000000¤000000000¤000000000¤000000000¤
000002156B211728153A211729079F000000000¤000000000¤000000000¤000000000¤000000000¤
000004157A101726158F101727196C101728196G101729197A000000000¤000000000¤000000000¤
000001158F211726157I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000004159F101701198H101702198I101703199C101704199D000000000¤000000000¤000000000¤
000005194E651202194F151947800B490001079I241929194I690443119G000000000¤000000000¤
000000195B691953195D000000161¤241999199F000000000¤000000000¤000000000¤000000000¤
000000195B691953195D000002000¤241998199F000000000¤000000000¤000000000¤000000000¤
000001196C211727158¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001196G211728158A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001197A211729079F000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001197B211701145D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000003197D211702145E211703145F211704199I000000000¤000000000¤000000000¤000000000¤
000002197I211701150D211702150E000000000¤000000000¤000000000¤000000000¤000000000¤
000001198B211703150F000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001198E211704199I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000002198H211701155D211702155E000000000¤000000000¤000000000¤000000000¤000000000¤
000002199C211703030D211704199I000000000¤000000000¤000000000¤000000000¤000000000¤
000001085C460802081I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001062B690825103G000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001103G241378069I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001103H460891074B000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001057B160625103H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
```

X. APPENDIX D: STRUCTURE FACTORS

The observed and calculated structure factor amplitudes for the erbium, yttrium and praseodymium ethylsulfates are given in Tables 25, 26 and 27 respectively of this appendix. An L is inserted in the value of F_o for unobserved reflections to indicate that the value given is that for F_{min}. If F_o is left blank, the reflection intensity was not measured.

TABLE 25. STRUCTURE FACTORS FOR ERBIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES ≤ AND K = 1.2)

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
H	1	0	6	151	152	13	L49	9-	4	58	54-	H	11	0
0		226-	7	100	89-	14	68	58	5	130	142	0	121	107-
1		192	8	107	104-	15	L53	20-	6	45	45-	1	80	74-
2		20-	9	110	112	16	L55	21-	7	42	37-	2	96	104
3	131	125-	10	55	62-	H	6	0	8	130	121	3	93	98-
4	206	207	11	58	64-	0	327	304	9	56	47-	4	43	49-
5	77	79-	12	85	100	1	311	293-	10	L48	21-	5	87	105
6	135	133-	13	L46	30-	2	L29	8	11	66	74	6	52	41-
7	368	358	14	63	78-	3	183	178	12	L52	12-	7	48	28-
8	46	38-	15	84	110	4	85	84-	13	L54	23-	8	75	77
9	137	131-	16	L52	23-	5	129	126-	14	L56	53	9	L52	14-
10	148	171	17	L55	44-	6	60	79	15	L58	22-	10	L53	18-
11	78	77-	18	69	68	7	63	58-	16	L59	28-	11	L56	54
12	58	56-	H	4	0	8	90	93-	H	9	0	12	L56	15-
13	81	99	0	187	172-	9	116	127	0	206	191	H	12	0
14	64	67-	1	256	237	10	54	63-	1	69	77-	0	123	131
15	63	63-	2	220	204-	11	77	81-	2	51	42-	1	68	61-
16	75	94	3	68	69-	12	94	106	3	110	104	2	59	61-
17	52	49-	4	180	183	13	L51	35-	4	67	67-	3	69	77
H	2	0	5	61	47	14	L53	41-	5	70	71-	4	75	68-
0		176-	6	187	190-	15	82	91	6	85	100	5	78	73-
1		288-	7	140	147	16	L56	25-	7	73	77-	6	59	69
2	80	82	8	L36	22-	H	7	0	8	69	70-	7	50	45-
3	208	195-	9	64	56-	0	182	169-	9	87	106	8	52	41-
4	95	80-	10	116	128	1	212	238	10	66	64-	9	66	66
5	227	250	11	64	69-	2	95	91-	11	57	49-	10	68	52-
6	173	166-	12	64	66-	3	175	176-	12	66	81	11	L57	20-
7	161	160-	13	67	81	4	222	242	13	L56	34-	12	72	52
8	215	237	14	65	57-	5	L36	27-	14	L58	26-	H	13	0
9	156	152-	15	52	53-	6	152	147-	15	L58	65	0	42	35-
10	38	37-	16	L53	51	7	148	156	16	73	26-	1	126	133
11	125	147	H	5	0	8	87	78-	H	10	0	2	45	50-
12	94	94-	0	43	31	9	93	94-	0	119	109-	3	L46	19-
13	L33	1-	1	194	197-	10	124	129	1	204	210	4	130	128
14	96	108	2	172	176	11	63	58-	2	89	79-	5	49	43-
15	65	66-	3	89	90-	12	71	65-	3	L39	11	6	51	36-
16	L52	29-	4	110	101-	13	52	56	4	157	171	7	69	90
17	53	66	5	192	199	14	L55	39-	5	67	69-	8	L53	40-
H	3	0	6	113	112-	15	L57	41-	6	62	73-	H	14	0
0	391	446	7	L36	12-	16	L57	52	7	137	146	0	80	76-
1	280	267-	8	167	177	H	8	0	8	L48	56-	1	79	76-
2	190	153	9	73	90-	0	79	66-	9	L50	51-	2	90	94
3	232	256	10	L43	8	1	211	211-	10	73	80	3	48	35-
4	226	218-	11	95	103	2	192	200	11	L54	46-	4	50	52-
5	28	11	12	47	28-	3	107	99-	12	L55	30-	5	L51	62

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
6	L53	6-	9	164	153	11	76	70	H	6	1	11	L42	16
7	L54	40-	10	L30	10	12	L37	11	0	L22	17-	12	53	63-
8	62	68	11	152	153-	13	118	97-	1	250	264-	13	56	61
H	15	0	12	156	156	14	L40	43	2	154	153	14	L47	15
0	99	101	13	L36	16	15	L43	6-	3	29	26	H	9	1
1	48	47-	14	116	113-	16	77	67-	4	120	119-	0	37	32
2	69	56-	15	122	114	17	52	52	5	111	113	1	151	145-
3	66	75	16	L42	2-	18	48	2	6	L30	16	2	141	152
4	52	40-	17	94	91-	H	4	1	7	100	96-	3	54	50
5	65	53-	18	69	65	0	135	149	8	72	66	4	104	111-
6	54	52	19	48	10-	1	23	35-	9	L35	6	5	99	91
7	L56	39-	20	69	52-	2	53	60-	10	123	118-	6	44	38
H	16	0	21	50	40	3	109	128	11	48	66	7	122	120-
0	49	19-	H	2	1	4	99	94-	12	41	2	8	62	62
1	106	108	0		325-	5	150	161-	13	91	84-	9	L40	15
2	62	47-	1	210	273	6	179	196	14	44	44	10	82	84-
3	52	19-	2	176	174	7	105	81	15	L35	1	11	48	46
4	53	71	3	238	276-	8	142	134-	16	48	54-	12	72	3
5	L55	26-	4	263	309	9	173	167	H	7	1	13	53	67-
6	L57	22-	5	L22	24-	10	L35	14	0	85	79	14	54	48
7	57	52	6	258	282-	11	111	110-	1	61	34	H	10	1
H	17	0	7	128	137	12	125	126	2	175	179-	0	126	122
0	51	46-	8	35	27-	13	L40	12-	3	121	122	1	30	21-
1	52	53-	9	216	221-	14	73	72-	4	L29	20	2	140	141-
2	53	69	10	149	142	15	85	84	5	166	161-	3	127	119
3	L54	28-	11	L34	6	16	L45	16-	6	163	166	4	L35	4
4	L56	38-	12	104	98-	17	53	57-	7	L34	16	5	107	97-
5	64	63	13	94	84	18	48	48	8	94	101-	6	104	101
H	18	0	14	L39	3	H	5	1	9	139	139	7	L39	8-
0	92	88	15	66	68-	0	294	332-	10	L39	6-	8	67	55-
1	54	37-	16	81	67	1	282	316	11	58	60-	9	92	89
2	55	31-	17	L45	15	2	32	33-	12	100	91	10	L44	5-
3	56	58	18	47	41-	3	220	249-	13	L44	19-	11	L45	42-
H	19	0	19	48	40	4	234	248	14	L46	55-	12	53	54
0	55	17-	H	3	1	5	30	24-	H	8	1	13	48	14-
1	56	51	0	140	151	6	211	219-	0	195	196-	H	11	1
H	1	1	1	144	159-	7	160	156	1	195	195	0	134	125-
0		263	2	209	231	8	54	40-	2	49	38-	1	124	114
1		292-	3	L21	24	9	104	104-	3	148	141-	2	63	52-
2		319-	4	128	128-	10	102	96	4	145	161	3	112	107-
3	128	142	5	155	165	11	L38	4-	5	58	54-	4	95	90
4	L19	3-	6	71	54	12	85	74-	6	121	126-	5	38	35-
5	287	318-	7	62	57-	13	85	78	7	103	103	6	88	82-
6	139	149	8	104	104	14	44	16	8	37	17-	7	79	79
7	31	18	9	71	42-	15	50	52-	9	98	105-	8	47	24-
8	187	177-	10	102	92-	16	52	54	10	86	90	9	72	72-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
10	L45	60	1	L42	7-	13	100	102-	H	4	2	7	121	121
11	L47	6	2	53	51-	14	43	47	0	137	141	8	85	75
H	12	1	3	67	64	15	71	63	1	350	373-	9	104	105-
0	L34	28	4	30	1-	16	53	73-	2	L23	18	10	66	65
1	100	92-	5	52	47-	17	60	43	3	146	155	11	73	64
2	138	133	H	17	1	18	L51	28	4	242	271-	12	102	97-
3	L37	31	0	65	64-	H	2	2	5	L28	14-	13	47	57
4	110	104-	1	54	47	0		209	6	100	98	14	L49	29
5	116	104	2	12	1-	1	253	292	7	191	183-	15	93	85-
6	41	27	3	57	61-	2	196	227-	8	L35	18	H	7	2
7	88	86-	4	53	44	3	123	129	9	82	78	0	129	121
8	66	65	5	48	3-	4	170	175	10	152	153-	1	162	148-
9	45	3	H	18	1	5	203	219-	11	L40	34	2	45	40
10	78	75-	0	L32	1	6	111	105	12	90	81	3	132	126
11	53	49	1	61	58-	7	65	60	13	98	95-	4	246	295-
H	13	1	2	78	70	8	148	156-	14	77	66	5	96	86
0	90	77	3	48	3-	9	85	88	15	L48	43	6	98	98
1	36	8	4	L49	48-	10	74	68	16	57	59-	7	156	152-
2	113	102-	5	55	49	11	175	170-	17	L52	27	8	66	56
3	112	107	H	19	1	12	53	53	H	5	2	9	66	64
4	40	10	0	L47	46	13	L42	21	0	162	174	10	108	110-
5	69	68-	1	L48	1	14	106	104-	1	202	218	11	56	56
6	74	72	2	54	47-	15	46	52	2	130	120-	12	47	48
7	L44	7	H	20	1	16	48	17	3	146	145	13	55	66-
8	L45	39-	0	54	52-	17	56	62-	4	50	44	H	8	2
9	62	56	1	L49	36	18	L52	36	5	177	170-	0	96	76
10	54	3	2	49	2	H	3	2	6	200	189	1	106	109
H	14	1	H	21	1	0	226	263-	7	L34	4-	2	87	72-
0	82	84-	0	L50	2-	1	67	73	8	172	160-	3	130	120
1	61	58	1	50	30-	2	253	271	9	57	57	4	46	55
2	56	26-	H	0	2	3	293	324-	10	L40	32	5	106	106-
3	71	74-	0		582-	4	123	126	11	125	107-	6	42	34
4	L42	51	H	1	2	5	149	142	12	L44	33	7	39	41
5	48	13-	0		4	6	160	170-	13	L46	8	8	58	65-
6	74	67-	1		137-	7	166	164	14	77	72-	9	L43	26
7	46	47	2	66	44-	8	130	121	15	L50	36	10	L45	28
8	53	3-	3	148	176	9	142	136-	16	L52	20	11	67	73-
H	15	1	4	288	312-	10	88	78	17	54	50-	12	L49	25
0	L39	20	5	L24	26	11	124	108	H	6	2	13	L51	27
1	105	88-	6	50	46	12	106	101-	0	212	239-	H	9	2
2	114	100	7	169	179-	13	43	39	1	155	143	0	100	106-
3	L43	10	8	63	39-	14	60	65	2	36	36	1	36	11
4	93	81-	9	77	82	15	86	88-	3	195	207-	2	37	38
5	L45	66	10	124	122-	16	L49	25	4	176	172	3	150	146-
H	16	1	11	L36	36	17	51	47	5	89	88	4	48	54
0	80	73	12	103	97	18	59	65-	6	139	141-	5	86	70

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
6	94	89-	9	84	72-	6	L53	16	0		246	8	98	90
7	46	57	10	52	41	7	L54	39-	1	113	132-	9	151	149-
8	43	39	11	L54	28	8	56	27	2	58	57-	10	L34	17-
9	78	79-	H	13	2	H	17	2	3	217	246	11	98	86
10	62	53	0	74	68	0	L48	29	4	127	144-	12	110	107-
11	59	47	1	157	147-	1	L49	41	5	L22	6	13	L19	1
12	88	81-	2	46	57	2	67	66-	6	244	266	14	78	64
13	52	28	3	48	34	3	L51	24	7	57	65-	15	83	78-
H	10	2	4	146	131-	4	58	38	8	L28	5	16	L45	8
0	140	126	5	92	74	5	66	64-	9	217	233	17	57	55
1	212	206-	6	L47	20	6	L55	19	10	119	122-	H	5	3
2	72	64	7	92	86-	7	L56	19	11	L34	11-	0	242	277
3	69	55	8	57	44	8	63	47-	12	122	116	1	191	218-
4	201	195-	9	L52	34	H	18	2	13	83	86-	2	42	30
5	64	66	10	L54	51-	0	67	66-	14	43	6	3	224	236
6	63	57	11	L55	28	1	L51	27	15	65	64	4	180	182-
7	125	116-	H	14	2	2	L52	43	16	67	64-	5	42	33
8	56	49	0	66	59	3	65	61-	17	44	7-	6	212	221
9	46	41	1	67	73	H	19	2	H	3	3	7	134	131-
10	69	75-	2	83	84-	0	L52	14	0	84	101-	8	50	38
11	L50	35	3	51	30	1	53	51-	1	70	78	9	128	121
12	L52	37	4	L46	44	H	20	2	2	167	203-	10	94	88-
H	11	2	5	59	73-	0	54	30	3	91	76-	11	L37	11
0	119	103	6	L49	23	H	1	3	4	86	92	12	81	79
1	100	92	7	57	37	0		193-	5	160	149-	13	84	76-
2	100	98-	8	78	70-	1		42	6	78	62-	14	42	3-
3	58	55	9	L54	12	2	231	316	7	43	48	15	50	49
4	102	90	10	L55	31	3	211	246-	8	98	100-	H	6	3
5	95	91-	11	62	48-	4	46	42-	9	L31	24	0	L22	17-
6	44	32	H	15	2	5	231	269	10	104	91	1	113	134
7	L46	32	0	69	70-	6	187	215-	11	74	67-	2	119	117-
8	70	72-	1	L45	25	7	L25	3-	12	L36	13-	3	92	77-
9	L48	12	2	52	48	8	98	105	13	112	91	4	93	87
10	50	39	3	67	73-	9	159	160-	14	L40	40-	5	127	120-
11	74	62-	4	73	49	10	L30	9-	15	L42	6	6	54	43-
12	54	15	5	56	46	11	110	110	16	69	63	7	98	90
H	12	2	6	63	58-	12	144	142-	17	L45	47-	8	84	78-
0	154	146-	7	L53	39	13	L36	25-	H	4	3	9	L35	17-
1	L38	29	8	L54	23	14	87	91	0	145	170-	10	118	105
2	109	91	H	16	2	15	103	99-	1	L18	6-	11	82	72-
3	119	99-	0	L46	10	16	L42	6-	2	168	170	12	L25	1-
4	57	51	1	82	85-	17	92	79	3	185	193-	13	79	74
5	73	63	2	68	55	18	55	60-	4	100	107	14	49	48-
6	79	77-	3	L49	11	19	L47	5	5	140	138	15	L32	1
7	53	49	4	72	69-	20	54	49	6	205	214-	H	7	3
8	L49	37	5	52	36	H	2	3	7	41	28-	0	81	81-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
1	L25	19	14	67	45-	5	58	63	H	19	3	13	L43	4-
2	191	185	H	10	3	6	82	64-	0	51	47-	14	106	96
3	139	130-	0	104	105-	7	L43	4-	1	L47	4-	15	57	51-
4	54	41	1	48	43	8	L45	39	2	L47	46	H	3	4
5	149	133	2	133	139	9	L46	50-	3	54	44-	0	163	222
6	152	143-	3	112	101-	10	L47	4-	H	20	3	1	111	125-
7	L34	8	4	L34	13	H	14	3	0	47	47	2	37	28-
8	81	75	5	93	87	0	64	63	1	L48	30-	3	160	188
9	99	106-	6	90	76-	1	60	60-	H	21	3	4	140	149-
10	L38	4	7	38	13	2	39	24	0	48	1	5	76	80-
11	49	53	8	49	49	3	40	55	1	L49	29	6	133	147
12	78	78-	9	66	69-	4	41	48-	H	0	4	7	117	111-
13	L43	12	10	L43	2	5	47	9	0		617	8	107	103-
14	L45	54	11	44	46	6	69	56	H	1	4	9	107	104
15	57	54-	H	11	3	7	45	44-	0		125-	10	95	82-
H	8	3	0	103	99	8	46	2-	1		219	11	63	52-
0	143	153	1	122	127-	9	L47	45	2		42-	12	69	77
1	178	178-	2	38	41	10	68	45-	3	37	46-	13	L44	38-
2	28	35	3	103	87	H	15	3	4	160	179	14	65	59-
3	136	125	4	103	88-	0	L38	20-	5	53	54-	15	83	82
4	158	151-	5	42	26	1	98	91	6	63	57-	H	4	4
5	64	49	6	70	65	2	100	89-	7	210	229	0	89	92-
6	106	115	7	70	72-	3	L42	5-	8	31	15-	1	175	214
7	90	90-	8	L42	17	4	91	81	9	97	91-	2	79	83-
8	L37	17	9	74	64	5	70	65-	10	135	123	3	40	43-
9	94	95	10	50	56-	6	L45	5	11	46	46-	4	167	178
10	90	81-	11	L46	9-	7	57	55	12	56	59-	5	53	42
11	L42	10-	H	12	3	H	16	3	13	90	84	6	117	118-
12	57	60	0	60	40-	0	70	68-	14	53	51-	7	147	137
13	50	56-	1	113	104	1	L42	2	15	60	60-	8	L36	7-
14	L46	10-	2	119	114-	2	L42	47	16	79	82	9	59	45-
H	9	3	3	45	41-	3	72	63-	17	56	44-	10	115	114
0	72	57-	4	123	112	4	L27	1	H	2	4	11	46	47-
1	112	107	5	110	104-	5	46	43	0		174-	12	48	56-
2	106	116-	6	L40	20-	H	17	3	1	123	159-	13	78	76
3	98	84-	7	102	83	0	L42	49	2	111	128	14	L47	46-
4	114	116	8	75	67-	1	48	39-	3	156	173-	15	69	44-
5	103	94-	9	L43	1	2	L10	1	4	39	37-	H	5	4
6	50	50-	10	73	68	3	50	52	5	157	175	0	100	107-
7	129	112	11	58	47-	4	L46	38-	6	128	119-	1	109	119-
8	77	70-	H	13	3	H	18	3	7	92	88-	2	113	107
9	L40	13-	0	81	73-	0	L05	1	8	153	175	3	120	118-
10	66	75	1	L36	6-	1	55	57	9	99	98-	4	81	60-
11	48	51-	2	118	96	2	65	64-	10	36	28-	5	108	114
12	L44	2-	3	118	94-	3	L46	4	11	137	126	6	87	85-
13	65	57	4	L39	4-	4	47	47	12	65	65-	7	L35	21-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
8	134	125	8	104	92	0	112	111	5	76	56	H	3	5
9	67	61-	9	L44	37-	1	L39	40-	H	18	4	0	38	49
10	L41	10-	10	L46	31-	2	46	45-	0	80	69	1	96	112-
11	96	89	11	53	66	3	69	73	1	57	29-	2	122	154
12	L45	24-	12	L49	16-	4	53	49-	H	19	4	3	L27	2-
13	L46	15-	H	9	4	5	71	56-	0	L52	14-	4	70	80-
14	59	56	0	148	165	6	56	65	1	53	45	5	121	120
H	6	4	1	52	47-	7	47	35-	H	20	4	6	L34	29
0	194	222	2	L35	31-	8	49	33-	0	60	27-	7	61	56-
1	148	158-	3	111	107	H	13	4	H	1	5	8	87	79
2	L28	33-	4	59	53-	0	49	48-	0		175	9	L41	26-
3	161	165	5	55	52-	1	121	119	1		128-	10	69	68-
4	90	80-	6	96	93	2	60	59-	2	119	175-	11	51	56
5	107	106-	7	66	64-	3	L44	20-	3	90	106	12	L48	3
6	94	92	8	62	50-	4	114	105	4	25	23-	13	80	73-
7	66	72-	9	103	88	5	L46	47-	5	176	183-	14	53	38
8	75	71-	10	58	52-	6	54	27-	6	115	116	15	L55	3-
9	104	104	11	L49	38-	7	L49	70	7	L33	12	H	4	5
10	60	64-	12	72	67	8	L51	35-	8	129	136-	0	75	96
11	70	59-	H	10	4	H	14	4	9	124	121	1	43	37-
12	74	81	0	121	116-	0	47	55-	10	L40	9	2	71	67-
13	48	32-	1	172	185	1	53	59-	11	114	111-	3	90	93
H	7	4	2	98	73-	2	81	78	12	109	114	4	L31	45-
0	147	139-	3	L37	11-	3	L46	25-	13	L48	9	5	122	118-
1	201	206	4	144	151	4	L48	46-	14	94	87-	6	116	130
2	47	49-	5	76	68-	5	L48	57	15	91	87	7	54	50
3	138	132-	6	52	54-	6	L50	5-	16	L55	2-	8	105	100-
4	199	216	7	131	119	7	L51	36-	17	80	71-	9	127	123
5	39	26-	8	56	50-	8	75	61	H	2	5	10	46	5
6	109	102-	9	L48	38-	H	15	4	0		205-	11	86	81-
7	137	141	10	60	66	0	80	79	1	132	180	12	96	95
8	76	60-	11	51	36-	1	65	33-	2	64	70	13	L52	8-
9	76	68-	H	11	4	2	74	48-	3	153	177-	14	66	58-
10	113	110	0	97	90-	3	58	65	4	170	190	15	63	64
11	56	45-	1	46	55-	4	L49	30-	5	L30	13-	H	5	5
12	58	50-	2	66	70	5	L50	46-	6	193	195-	0	177	199-
13	49	53	3	75	69-	H	16	4	7	117	113	1	183	207
H	8	4	4	L41	50-	0	L46	20-	8	L37	17-	2	L30	21-
0	114	108-	5	77	80	1	107	91	9	145	153-	3	171	170-
1	120	132-	6	45	30-	2	L48	48-	10	125	105	4	165	164
2	127	110	7	L46	36-	H	17	4	11	L45	2-	5	L36	12-
3	91	87-	8	76	67	0	L48	36-	12	66	72-	6	154	153-
4	56	50-	9	L49	16-	1	L49	42-	13	69	66	7	118	110
5	76	86	10	L51	22-	2	62	62	14	52	2	8	48	26-
6	43	32-	11	64	49	3	L52	22-	15	L54	55-	9	78	80-
7	57	48-	H	12	4	4	L53	31-	16	62	54	10	75	76

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
11	L49	3-	0	36	21	2	73	77-	4	118	120	5	136	137-
12	52	58-	1	109	110-	3	80	81	5	137	144-	6	116	110
13	54	59	2	113	113	4	L52	7	6	98	81	7	L46	7
H	6	5	3	L41	31	5	60	54-	7	64	60	8	118	117-
0	L29	4-	4	78	82-	H	14	5	8	117	119-	9	L52	50
1	152	161-	5	75	72	0	69	66-	9	80	75	10	54	16
2	119	118	6	L47	25	1	70	50	10	48	45	11	70	75-
3	38	21	7	91	93-	2	L52	18-	11	116	111-	12	L59	28
4	81	88-	8	71	54	3	64	59-	12	66	47	H	6	6
5	77	80	9	L53	10	4	L54	41	13	L57	18	0	139	150-
6	L40	18	10	77	67-	H	15	5	14	84	70-	1	98	105
7	77	76-	11	63	38	0	L51	14	H	3	6	2	L38	12
8	50	54	H	10	5	1	79	69-	0	162	222-	3	105	115-
9	L47	3	0	90	92	2	85	77	1	80	96	4	102	94
10	100	89-	1	L40	11-	3	55	8	2	59	63	5	50	50
11	57	52	2	101	102-	4	69	62-	3	166	190-	6	87	84-
12	L53	3	3	90	90	H	16	5	4	90	90	7	78	63
13	78	65-	4	24	1	0	76	60	5	L37	39	8	63	56
H	7	5	5	75	74-	1	L55	5-	6	102	103-	9	77	77-
0	73	73	6	78	81	2	56	44-	7	67	76	10	L57	38
1	L33	15	7	57	5-	H	17	5	8	64	64	11	L59	50
2	119	132-	8	53	47-	0	56	53-	9	96	89-	12	97	75-
3	86	90	9	86	70	H	0	6	10	L51	34	H	7	6
4	L38	18	H	11	5	0		349-	11	84	71	0	72	77
5	120	115-	0	89	93-	H	1	6	12	89	79-	1	94	108-
6	131	118	1	91	89	0		64	13	83	22	2	L40	42
7	L45	12	2	L45	40-	1		78-	H	4	6	3	73	80
8	81	81-	3	72	78-	2		6	0	92	107	4	157	164-
9	114	107	4	58	71	3	94	108	1	135	167-	5	L46	53
10	51	5-	5	L49	25-	4	130	154-	2	35	41	6	78	72
11	L53	50-	6	72	66-	5	L32	15	3	94	104	7	106	99-
12	61	70	7	75	62	6	81	64	4	135	148-	8	L53	42
H	8	5	8	55	16-	7	117	132-	5	L39	15	9	63	52
0	132	146-	H	12	5	8	L41	2	6	92	81	10	72	76-
1	155	150	0	L43	19	9	54	63	7	116	118-	H	8	6
2	L37	28-	1	51	70-	10	97	99-	8	47	29	0	L40	32
3	114	109-	2	102	100	11	L50	39	9	71	60	1	83	86
4	106	115	3	L48	18	12	64	57	10	98	98-	2	99	96-
5	L42	35-	4	79	77-	13	67	74-	11	L54	35	3	72	71
6	97	97-	5	78	77	14	65	38	12	71	54	4	L47	40
7	81	82	6	L53	20	15	60	38	H	5	6	5	99	97-
8	L49	12-	7	61	67-	H	2	6	0	34	43	6	L51	35
9	84	83-	8	56	51	0		68	1	116	128	7	L53	19
10	87	71	H	13	5	1	103	141	2	117	116-	8	55	60-
11	L55	11	0	52	62	2	94	119-	3	70	70	9	L58	24
H	9	5	1	L48	3	3	58	69	4	63	55	H	9	6

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
0	77	74-	H	14	6	8	58	65-	2	85	94	2	39	30-
1	L44	33	0	L57	47	9	L55	11	3	78	76-	3	L32	37-
2	L46	35	1	L58	52	10	66	64	4	L51	3	4	72	100
3	79	85-	H	15	6	11	L62	47-	5	90	86	5	48	26-
4	L50	44	0	L59	60-	12	L65	8-	6	106	93-	6	43	36-
5	64	54	1	L60	26	H	4	7	7	L60	3-	7	101	111
6	60	61-	H	16	6	0	70	84-	8	62	56	8	50	14-
7	L55	41	0	L62	10	1	L34	11	9	79	74-	9	66	48-
8	L58	36	1	70	61-	2	88	89	H	8	7	10	82	73
9	74	60-	H	1	7	3	69	81-	0	88	91	11	L61	28-
H	10	6	0		99-	4	L43	26	1	97	101-	12	71	37-
0	51	59	1		63	5	79	92	2	L50	21	H	2	8
1	123	129-	2	85	131	6	104	110-	3	102	84	0		74-
2	L48	39	3	78	93-	7	L51	20-	4	78	93-	1	47	76-
3	L51	35	4	L34	2	8	86	77	5	L57	27	2	62	85
4	118	122-	5	128	133	9	92	94-	6	66	73	3	71	81-
5	L54	38	6	81	89-	10	L61	11-	H	9	7	4	L39	40-
6	63	45	7	44	8-	11	63	67	0	L50	18-	5	86	98
7	83	83-	8	83	83	12	74	73-	1	73	74	6	65	64-
H	11	6	9	100	86-	H	5	7	2	75	81-	7	55	44-
0	54	65	10	L54	10-	0	118	146	3	L55	29-	8	102	96
1	71	66	11	92	85	1	124	142-	4	58	71	9	62	52-
2	81	85-	12	92	87-	2	L40	3	5	L59	59-	10	L60	21-
3	L53	46	H	2	7	3	127	132	H	10	7	11	69	77
4	L54	52	0		134	4	114	124-	0	53	64-	H	3	8
5	70	73-	1	85	120-	5	L48	22	1	L54	6	0	86	127
6	59	29	2	55	56-	6	121	116	2	98	85	1	44	65-
7	L60	18	3	139	153	7	102	91-	3	66	69-	2	L35	33-
H	12	6	4	120	124-	8	L57	19	4	L61	5-	3	82	110
0	96	95-	5	L40	3-	9	85	70	5	63	60	4	66	73-
1	L52	32	6	136	138	10	70	59-	H	11	7	5	50	49-
2	77	63	7	L47	74-	H	6	7	0	79	70	6	78	87
3	79	68-	8	50	10	0	L39	3-	1	58	72-	7	58	62-
4	64	42	9	108	115	1	96	100	2	L59	19	8	55	56-
5	59	46	10	79	78-	2	79	84-	3	69	68	9	L58	66
6	L62	54-	11	66	7-	3	L46	16-	H	12	7	10	61	47-
7	L63	38	12	62	67	4	69	67	0	L59	16-	H	4	8
H	13	6	H	3	7	5	93	78-	1	74	64	0	58	57-
0	L53	33	0		25-	6	L54	6-	2	70	75-	1	94	113
1	107	96-	1	90	94	7	70	60	H	13	7	2	L39	35-
2	L57	29	2	102	115-	8	L59	47-	0	62	53-	3	L42	40-
3	L58	25	3	L36	24-	9	62	5-	H	0	8	4	98	104
4	112	91-	4	57	75	10	65	67	0		224	5	L48	3
5	76	42	5	92	93-	H	7	7	H	1	8	6	57	59-
6	L64	20	6	L46	16-	0	65	49-	0		61-	7	94	85
7	80	65-	7	L50	44	1	L44	4-	1		107	8	L57	13-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
9	L61	33-	2	L56	24-									
H	5	8	3	58	68									
0	54	63-	4	L61	34-									
1	57	65-	5	L63	34-									
2	68	72	6	L65	59									
3	68	66-	7	L68	37-									
4	48	38-	8	L69	29-									
5	72	72	H	10	8									
6	61	50-	0	68	61-									
7	L57	19-	1	100	103									
8	L60	73	2	L60	43-									
9	L62	35-	3	L61	18-									
H	6	8	4	90	88									
0	96	116	5	L65	40-									
1	54	71-	6	L68	32-									
2	L46	26-	7	L70	71									
3	78	93	8	80	30-									
4	62	50-	H	11	8									
5	61	54-	0	65	50-									
6	64	64	1	L61	36-									
7	L60	45-	H	12	8									
8	L62	41-	0	62	67									
9	72	63	1	L64	25-									
H	7	8	H	13	8									
0	72	71-	0	L65	31-									
1	114	111	1	94	72									
2	L50	29-												
3	51	66-												
4	127	117												
5	L57	22-												
6	L60	54-												
7	76	83												
8	L65	34-												
H	8	8												
0	78	60-												
1	50	64-												
2	60	66												
3	L55	50-												
4	L57	33-												
5	L60	55												
6	L63	24-												
7	L65	30-												
8	L68	56												
H	9	8												
0	90	89												
1	L54	30-												

TABLE 26. STRUCTURE FACTORS FOR YTTRIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES ≤ AND K = 1.2)

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
H	1	0	12	36	25	1	122	134	5	36	31	8	40	20-
0		161-	13	L12	1	2	27	36-	H	12	0	9	132	127-
1	58	54	H	4	0	3	116	117-	0	50	40	10	68	65
2	52	44	0	117	111-	4	126	136	1	L30	20-	11	L33	5
3	46	48-	1	96	102	5	L31	21	2	L28	20-	12	30	33-
4	80	84	2	145	143-	6	93	90-	3	L26	11	13	L25	22
5	26	23-	3	L22	7-	7	63	73	4	29	28-	H	3	1
6	63	74-	4	69	63	8	38	34-	5	33	33-	0	166	148
7	229	234	5	95	97	9	50	54-	H	13	0	1	40	45-
8	L28	8	6	122	131-	10	61	56	0	L26	1	2	122	120
9	74	77-	7	60	45	H	8	0	1	54	55	3	L21	13
10	74	75	8	L32	18	0	L27	10-	2	L24	14-	4	34	28-
11	40	34-	9	L32	17-	1	148	153-	3	L20	11	5	70	66
12	L30	11-	10	43	41	2	102	98	4	48	56	6	62	53
13	L27	24	11	38	28-	3	53	52-	H	14	0	7	L31	25
14	29	29-	12	24	32-	4	L32	8-	0	34	32-	8	L33	28
H	2	0	13	17	15	5	53	51	1	33	37-	9	48	37-
0	111	110-	H	5	0	6	L31	6-	2	28	26	10	33	21-
1	208	219-	0	87	93	7	29	4	H	15	0	11	L07	1-
2	67	42-	1	138	131-	8	53	49	0	40	37	12	L27	5
3	133	125-	2	54	60	H	9	0	H	1	1	13	53	33-
4	25	17-	3	31	33-	0	94	90	0		150	H	4	1
5	123	128	4	52	52-	1	41	35-	1		281-	0	37	39
6	104	107-	5	99	102	2	L31	9	2	179	199-	1	37	42-
7	100	107-	6	57	54-	3	L32	13	3	35	38	2	59	42
8	124	135	7	L31	28	4	40	33-	4	L20	3-	3	24	35
9	87	97-	8	84	82	5	30	31-	5	219	208-	4	79	84-
10	40	13	9	47	51-	6	L28	27	6	56	51	5	74	71-
11	60	62	10	35	36	7	40	37-	7	L28	18	6	98	101
12	45	50-	11	33	32	8	31	33-	8	96	88-	7	79	69
13	30	28	H	6	0	H	10	0	9	89	74	8	55	52-
14	45	42	0	183	187	0	69	57-	10	L34	14	9	88	87
H	3	0	1	241	223-	1	120	113	11	76	71-	10	L32	14
0	274	310	2	52	52	2	40	33-	12	77	78	11	46	43-
1	193	204-	3	73	75	3	42	44	13	L28	13	12	63	58
2	231	215	4	36	35-	4	73	79	14	52	49-	H	5	1
3	120	131	5	72	72-	5	L28	28-	H	2	1	0	238	230-
4	155	155-	6	L31	6-	6	31	31-	0	180	208-	1	195	201
5	52	48	7	L32	17-	7	76	68	1	157	157	2	35	28-
6	52	37	8	50	51-	H	11	0	2	180	173	3	145	146-
7	47	34-	9	38	48	0	55	60-	3	166	164-	4	151	147
8	50	48-	10	27	26-	1	35	31-	4	195	191	5	L31	22-
9	L32	27	11	43	40-	2	L31	20	5	L24	25-	6	128	131-
10	40	19-	H	7	0	3	54	53-	6	171	177-	7	83	68
11	L29	24-	0	117	106-	4	L27	12-	7	48	48	8	34	38-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
9	32	35-	0	42	41	12	61	52	12	49	41	6	L33	6-
10	37	34	1	L34	30-	13	47	30-	H	5	2	7	L27	1
H	6	1	2	55	58-	14	L19	11	0	109	121	H	9	2
0	L24	18-	3	42	44	H	2	2	1	153	148	0	L30	13-
1	147	156-	4	L32	2	0	121	148	2	L24	5-	1	31	28-
2	63	60	5	L29	29-	1	202	226	3	93	94	2	27	8-
3	L29	27	6	47	42	2	95	109-	4	L28	6-	3	45	55-
4	L31	35-	H	11	1	3	68	67	5	77	75-	4	L31	16
5	L33	31	0	55	49-	4	118	114	6	137	132	5	30	34
6	L34	10	1	43	40	5	102	98-	7	36	41-	6	L30	18-
7	L34	22-	2	41	45-	6	66	56	8	82	64-	7	L23	18
8	L11	1-	3	39	40-	7	L29	13	9	L30	21	H	10	2
9	L30	7	4	L28	27	8	72	62-	10	L26	1	0	81	78
10	51	48-	5	25	29-	9	57	38	11	49	36-	1	108	111-
H	7	1	6	28	23-	10	L32	26	H	6	2	2	L32	20
0	L26	16-	H	12	1	11	94	86-	0	119	123-	3	L31	25
1	43	35	0	L33	27	12	L27	13	1	89	75	4	94	104-
2	81	85-	1	L32	22-	13	L22	8-	2	L26	17-	5	29	27
3	44	39	2	65	62	14	41	40-	3	105	105-	6	L25	19
4	L33	18	3	L27	25	H	3	2	4	120	118	7	46	44-
5	76	74-	4	46	43-	0	141	133-	5	41	35	H	11	2
6	89	82	5	40	39	1	L17	12	6	39	55-	0	62	60
7	L33	13	H	13	1	2	198	208	7	74	71	1	38	47
8	38	36-	0	L30	12	3	188	204-	8	30	33	2	L30	21-
9	74	71	1	35	9	4	73	71	9	L27	28-	3	L28	15
H	8	1	2	50	37-	5	95	96	10	L22	26	4	46	48
0	111	97-	3	48	41	6	58	65-	11	17	24	5	L21	23-
1	106	107	H	14	1	7	111	112	H	7	2	H	12	2
2	45	38-	0	L25	22-	8	79	66	0	67	62	0	66	57-
3	61	63-	1	L22	5	9	70	54-	1	36	42-	1	L29	6-
4	74	79	2	32	22-	10	31	33	2	L29	13-	2	46	48
5	48	43-	H	0	2	11	73	65	3	70	75	3	39	31-
6	53	54-	0		435-	12	L24	27-	4	176	188-	4	L22	16
7	30	34	H	1	2	H	4	2	5	32	35	5	24	24
8	L26	16-	0		61-	0	83	78	6	57	49	H	13	2
9	44	43-	1	L11	8-	1	232	241-	7	62	67-	0	L30	29
H	9	1	2	124	109-	2	37	39-	8	L30	15	1	73	67-
0	40	36	3	102	105	3	90	90	9	L23	26	H	1	3
1	65	56-	4	193	195-	4	147	157-	10	38	39-	0		84-
2	67	68	5	38	33-	5	61	56-	H	8	2	1	28	37
3	34	41	6	L25	9-	6	L30	42	0	L28	22	2	177	205
4	L34	35-	7	77	67-	7	98	89-	1	57	55	3	136	144-
5	L32	20	8	95	81-	8	L32	18-	2	L31	20	4	36	39-
6	38	36	9	L31	34	9	L31	38	3	76	69	5	167	169
7	57	47-	10	48	40-	10	73	66-	4	L32	15	6	125	118-
H	10	1	11	L31	5-	11	L25	1-	5	L32	20-	7	L24	2-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
8	L26	24	8	L27	18	6	34	44	9	29	44-	3	72	66-
9	92	82-	9	79	71-	7	30	26-	10	49	44	4	L28	20-
10	L27	14-	10	L23	16-	H	9	3	11	L26	11-	5	L29	33
11	43	38	11	33	27	0	55	54-	12	L22	18-	6	42	35-
12	77	68-	H	5	3	1	L27	26	13	16	19	7	L29	14
13	L19	21-	0	174	182	2	39	37-	H	2	4	8	43	43
14	24	33	1	111	119-	3	72	71-	0	90	109-	9	L23	28-
H	2	3	2	31	23	4	45	44	1	78	100-	10	26	16
0	127	137	3	132	137	5	L24	25-	2	L18	22	H	6	4
1	29	27-	4	94	95-	6	30	45-	3	108	113-	0	128	123
2	62	62-	5	37	32	7	42	43	4	L23	8	1	97	101-
3	152	151	6	135	134	H	10	3	5	74	72	2	L27	12
4	48	45-	7	50	53-	0	L27	29-	6	77	70-	3	76	73
5	L22	5	8	L26	35	1	L27	36	7	56	45-	4	L29	33-
6	168	167	9	56	51	2	68	61	8	91	85	5	59	56-
7	L26	11	10	21	29-	3	44	32-	9	41	52-	6	L29	16
8	L27	2	H	6	3	4	L23	10	10	L27	11	7	L27	30-
9	142	142	0	L21	13-	5	29	25	11	55	50	8	34	34-
10	52	50-	1	32	37	H	11	3	H	3	4	9	L19	35
11	24	9-	2	24	31-	0	27	30	0	104	116	H	7	4
12	55	51	3	80	71-	1	53	56-	1	65	72-	0	98	86-
13	L16	26-	4	L26	11	2	L24	35	2	L20	31	1	106	111
H	3	3	5	50	44-	3	L22	26	3	82	84	2	L29	4-
0	79	95-	6	39	34-	4	L19	28-	4	98	96-	3	79	81-
1	22	19-	7	26	21	H	12	3	5	L27	35-	4	107	118
2	91	101-	8	L24	14-	0	35	35-	6	55	48	5	L29	14
3	73	69-	9	L21	16-	1	39	37	7	65	57-	6	60	55-
4	L21	2	10	41	40	2	41	46-	8	57	50-	7	55	64
5	71	59-	H	7	3	3	23	33-	9	L28	27	8	38	23-
6	62	60-	0	L23	9	4	53	53	10	L25	39-	9	20	33-
7	L27	27-	1	L24	15	H	13	3	H	4	4	H	8	4
8	L27	30-	2	97	95	0	L21	13-	0	39	44-	0	58	54-
9	L27	17	3	53	49-	1	L19	9-	1	99	99	1	79	83-
10	L25	25	4	47	37	2	39	34	2	23	34-	2	29	29
11	L22	3-	5	67	56	H	0	4	3	L25	5	3	41	45-
12	L18	8-	6	72	64-	0		489	4	75	75	4	L28	10-
13	30	30	7	L24	8	H	1	4	5	77	79	5	L26	12
H	4	3	8	L21	17	0		71-	6	65	69-	6	L24	1
0	63	67-	9	42	44-	1	79	98	7	57	50	7	L20	10-
1	L18	1	H	8	3	2	L16	13	8	L28	24	H	9	4
2	88	77	0	70	62	3	L19	9	9	L26	10-	0	76	75
3	103	100-	1	105	96-	4	66	74	10	32	37	1	L29	11-
4	94	98	2	L27	34	5	24	6-	H	5	4	2	L29	11
5	58	57	3	47	51	6	L26	13-	0	62	50-	3	28	24
6	131	121-	4	78	74-	7	131	127	1	61	66-	4	L26	22-
7	27	18-	5	26	38	8	L29	23	2	L25	15	5	L23	18-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
6	L19	26												
7	17	28-												
H	10	4												
0	70	66-												
1	85	94												
2	L27	33-												
3	L25	18												
4	61	68												
H	11	4												
0	56	46-												
1	L26	17-												
2	L24	3												
3	21	31-												
H	12	4												
0	35	31												
1	L22	6-												
H	13	4												
0	66	14-												
1	46	48												

TABLE 27. STRUCTURE FACTORS FOR PRASEODYMIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES ≤ AND K = 1.2)

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
H	1	0	7	84	79-	1	269	277-	3	84	80	7	77	92
0		201-	8	83	87-	2	L38	15	4	78	61-	8	83	45-
1		132	9	93	91	3	149	169	5	80	67-	H	14	0
2		2	10	61	56-	4	78	78-	6	94	91	0	73	75-
3	87	95-	11	66	63-	5	122	118-	7	75	80-	1	75	72-
4	173	182	12	81	93	6	51	57	8	71	66-	2	97	89
5	70	64-	13	L60	25-	7	62	55-	9	93	98	3	L63	29-
6	122	118-	14	74	81-	8	89	93-	H	10	0	4	68	52-
7	294	329	15	98	104	9	121	128	0	101	90-	5	L67	58
8	L42	32-	H	4	0	10	L58	54-	1	172	189	6	L69	4-
9	116	111-	0	167	159-	11	79	80-	2	90	73-	7	L71	38-
10	133	146	1	183	204	12	90	99	3	52	16	H	15	0
11	77	67-	2	183	187-	13	L67	30-	4	149	168	0	98	97
12	L54	41-	3	70	63-	14	L69	42-	5	70	66-	1	67	49-
13	91	89	4	146	162	15	87	96	6	68	70-	2	72	58-
14	77	67-	5	107	86	H	7	0	7	123	138	3	71	69
15	73	64-	6	170	179-	0	177	171-	8	L63	52-	4	68	41-
16	94	87	7	131	124	1	187	215	H	11	0	5	74	52-
17	80	48-	8	L48	15-	2	70	77-	0	101	91-	6	L72	53
18	75	21-	9	51	54-	3	160	167-	1	60	63-	7	80	44-
H	2	0	10	114	116	4	186	221	2	85	90	H	16	0
0		147-	11	64	57-	5	L48	19-	3	94	89-	0	L64	10-
1		260-	12	72	67-	6	147	140-	4	57	46-	1	99	107
2		40	13	70	75	7	136	153	5	90	90	2	67	49-
3	195	202-	14	79	53-	8	100	78-	6	L61	27-	3	L69	16-
4	88	70-	15	85	54-	9	94	92-	7	L63	21-	4	76	72
5	207	224	H	5	0	10	110	118	8	80	68	5	72	33-
6	141	141-	0	63	45	11	63	56-	H	12	0	H	17	0
7	144	149-	1	187	187-	H	8	0	0	108	107	0	L67	39-
8	196	215	2	145	151	0	70	57-	1	63	53-	1	68	54-
9	147	152-	3	75	69-	1	186	195-	2	70	63-	H	18	0
10	L50	24-	4	110	107-	2	173	179	3	72	70	0	90	80
11	117	129	5	173	173	3	110	103-	4	70	60-	1	75	38-
12	95	93-	6	107	106-	4	L48	33-	5	86	71-			
13	L57	1	7	L48	12	5	121	123	6	L64	60			
14	111	110	8	159	171	6	54	47-	7	L66	43-			
15	72	65-	9	85	85-	7	L55	27-	8	68	43-			
H	3	0	10	L56	9	8	116	117	H	13	0			
0		400	11	94	94	9	L60	40-	0	57	33-			
1	230	244-	12	L61	23-	10	L63	12-	1	120	138			
2	214	184	13	L64	5-	11	74	64	2	L58	49-			
3	204	226	14	71	55	H	9	0	3	L60	22			
4	184	183-	15	L70	22-	0	147	168	4	107	122			
5	L38	3	H	6	0	1	93	72-	5	64	36-			
6	126	122	0	256	273	2	L47	15-	6	L67	34-			